



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:01 AM UTC

PDB ID : 4NF9 / pdb_00004nf9
Title : Structure of the Knl1/Nsl1 complex
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muth, S.; Pasqualato, S.; Raunser, S.; Musacchio, A.
Deposited on : 2013-10-31
Resolution : 2.80 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

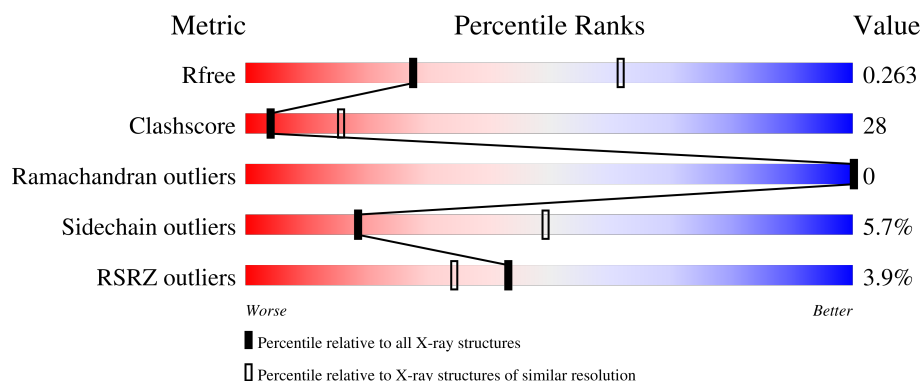
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	221	4% 57% 36% .
1	B	221	4% 56% 33% 5% 6%
2	C	26	15% 15% . 65%
2	D	26	35% 65%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3716 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 Protein CASC5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	Se	0	0	0
			1785	1153	285	343	2	2			
1	B	207	Total	C	N	O	S	Se	0	0	0
			1708	1106	272	326	2	2			

- Molecule 2 is a protein called Kinetochore-associated protein NSL1 homolog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			88	59	18	11			
2	D	9	Total	C	N	O	0	0	0
			88	59	18	11			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

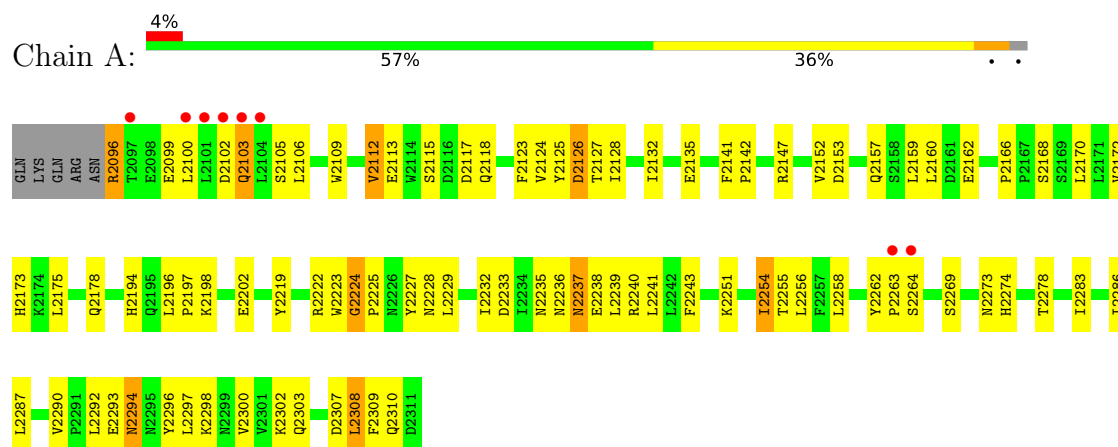
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	12	Total	O	0	0
			12	12		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

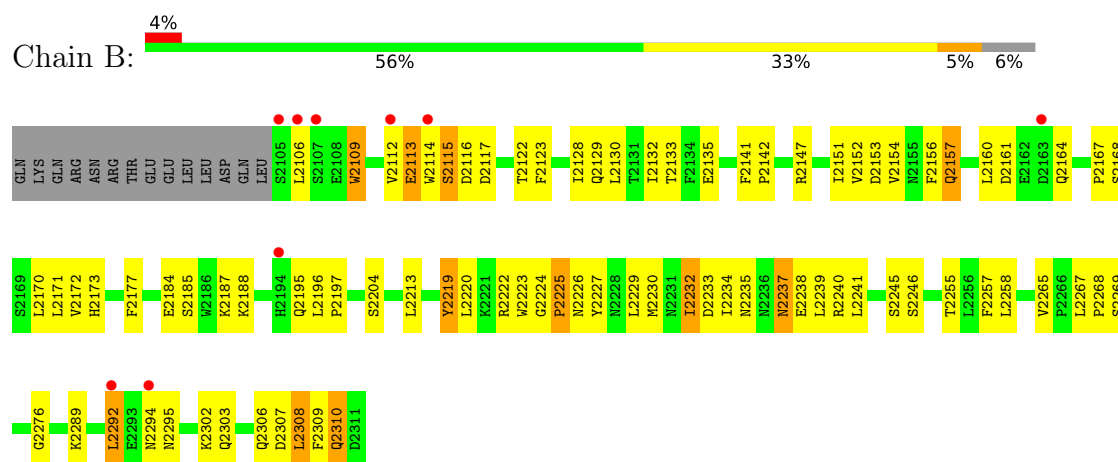
3 Residue-property plots

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.

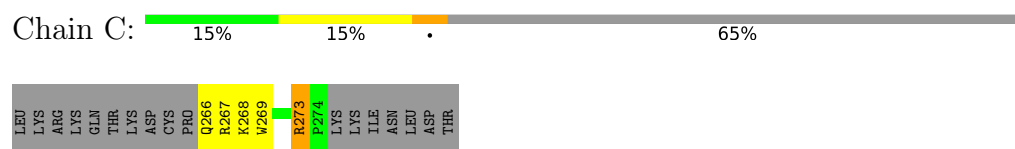
• Molecule 1: Protein CASC5



• Molecule 1: Protein CASC5



• Molecule 2: Kinetochores-associated protein NSL1 homolog



• Molecule 2: Kinetochores-associated protein NSL1 homolog



LEU	LYS	ARG	LYS	GLN	THR	LYS	ASP	CYS	PRO	Q266	Y274	LYS	LYS	ILE	ASN	LEU	ASP	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.71Å 71.63Å 177.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 2.80 46.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.31-2.80) 99.5 (46.31-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.265 0.207 , 0.263	Depositor DCC
R_{free} test set	983 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	1.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3716	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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:
CL

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	1.17	0/1826	1.22	3/2481 (0.1%)
1	B	1.07	0/1749	1.21	11/2377 (0.5%)
2	C	1.04	0/92	0.93	0/124
2	D	0.99	0/92	1.13	0/124
All	All	1.11	0/3759	1.21	14/5106 (0.3%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2117	ASP	N-CA-C	7.30	119.02	111.14
1	B	2276	GLY	N-CA-C	-6.77	105.14	112.04
1	A	2224	GLY	O-C-N	6.62	123.45	121.07
1	B	2115	SER	N-CA-C	6.13	118.82	110.35
1	B	2219	TYR	N-CA-C	-5.83	104.29	111.40
1	B	2265	VAL	CA-C-N	5.79	126.12	119.93
1	B	2265	VAL	C-N-CA	5.79	126.12	119.93
1	B	2230	MSE	CG-SE-CE	-5.72	86.33	98.92
1	B	2267	LEU	N-CA-C	5.61	117.03	109.24
1	A	2112	VAL	N-CA-CB	-5.55	105.72	112.33
1	B	2106	LEU	N-CA-C	5.43	117.70	110.53
1	B	2109	TRP	N-CA-C	5.36	118.02	110.14
1	B	2265	VAL	N-CA-C	5.28	113.65	107.89
1	B	2171	LEU	N-CA-C	-5.04	105.97	111.82

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	1785	0	1746	112	0
1	B	1708	0	1669	92	0
2	C	88	0	90	7	0
2	D	88	0	90	0	0
3	A	1	0	0	0	0
4	A	32	0	0	3	0
4	B	12	0	0	2	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	3716	0	3595	200	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 28.

All (200) 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:2307:ASP:C	1:A:2308:LEU:HD23	1.47	1.39
1:A:2262:TYR:CE1	1:A:2263:PRO:HB3	1.77	1.19
1:A:2307:ASP:O	1:A:2308:LEU:HD23	1.46	1.13
1:B:2307:ASP:C	1:B:2308:LEU:HD12	1.74	1.12
1:A:2105:SER:HB2	1:B:2114:TRP:HE1	1.13	1.12
1:B:2307:ASP:O	1:B:2308:LEU:HD12	1.56	1.05
1:B:2307:ASP:C	1:B:2308:LEU:CD1	2.30	1.04
1:A:2264:SER:O	1:A:2292:LEU:HD13	1.58	1.04
1:A:2100:LEU:O	1:A:2103:GLN:HG3	1.59	1.01
1:B:2310:GLN:HA	1:B:2310:GLN:OE1	1.60	0.97
1:A:2308:LEU:HD23	1:A:2308:LEU:N	1.67	0.96
1:B:2227:TYR:CE1	1:B:2302:LYS:HG2	2.00	0.96
1:B:2227:TYR:HE1	1:B:2302:LYS:HG2	1.28	0.96
1:B:2308:LEU:CD1	1:B:2308:LEU:N	2.30	0.95
1:A:2307:ASP:C	1:A:2308:LEU:CD2	2.40	0.91
1:B:2116:ASP:OD1	1:B:2117:ASP:N	2.03	0.91
1:B:2109:TRP:HB3	1:B:2123:PHE:CE1	2.08	0.88
1:A:2125:TYR:C	1:A:2126:ASP:OD1	2.17	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2262:TYR:CZ	1:A:2263:PRO:HB3	2.09	0.87
1:A:2099:GLU:HA	1:A:2102:ASP:OD2	1.75	0.86
1:A:2102:ASP:HB3	1:B:2147:ARG:NH2	1.91	0.86
1:A:2262:TYR:CD1	1:A:2263:PRO:HB3	2.10	0.85
1:A:2227:TYR:HE1	1:A:2302:LYS:HG2	1.41	0.84
1:B:2308:LEU:N	1:B:2308:LEU:HD13	1.95	0.80
1:A:2109:TRP:HB3	1:A:2123:PHE:CE1	2.17	0.80
1:A:2262:TYR:CD1	1:A:2263:PRO:HA	2.18	0.79
1:A:2115:SER:HB2	1:A:2118:GLN:H	1.46	0.79
1:A:2307:ASP:O	1:A:2308:LEU:CD2	2.30	0.79
1:B:2133:THR:HG22	1:B:2152:VAL:HG11	1.64	0.79
1:B:2310:GLN:OE1	1:B:2310:GLN:CA	2.30	0.79
1:A:2166:PRO:HG2	2:C:269:TRP:HE3	1.48	0.78
1:A:2105:SER:HB2	1:B:2114:TRP:NE1	1.95	0.78
1:A:2100:LEU:HA	1:A:2103:GLN:CG	2.15	0.77
1:A:2113:GLU:OE2	1:A:2115:SER:OG	2.03	0.76
1:A:2227:TYR:CE1	1:A:2302:LYS:HG2	2.20	0.76
1:B:2307:ASP:C	1:B:2308:LEU:HD13	2.10	0.76
1:A:2233:ASP:HB3	1:A:2240:ARG:HB2	1.67	0.76
1:A:2100:LEU:HA	1:A:2103:GLN:CD	2.11	0.75
1:B:2133:THR:HG22	1:B:2152:VAL:CG1	2.17	0.75
1:B:2133:THR:O	1:B:2152:VAL:HG12	1.86	0.75
1:A:2099:GLU:O	1:A:2102:ASP:HB2	1.86	0.75
1:A:2241:LEU:HB2	1:A:2254:ILE:HG23	1.69	0.74
1:A:2262:TYR:CE1	1:A:2263:PRO:CB	2.66	0.74
1:B:2160:LEU:HB2	1:B:2173:HIS:CE1	2.23	0.74
1:A:2286:ILE:HG23	1:A:2303:GLN:HG3	1.68	0.73
1:B:2245:SER:HB2	1:B:2309:PHE:CD1	2.26	0.71
1:A:2262:TYR:CD1	1:A:2263:PRO:CB	2.76	0.69
1:A:2099:GLU:O	1:A:2102:ASP:N	2.25	0.68
1:A:2237:ASN:ND2	1:A:2258:LEU:O	2.27	0.68
1:A:2262:TYR:CD1	1:A:2263:PRO:CA	2.76	0.67
1:B:2196:LEU:N	1:B:2197:PRO:HD2	2.10	0.66
1:A:2102:ASP:HB3	1:B:2147:ARG:CZ	2.26	0.65
1:A:2227:TYR:O	1:A:2228:ASN:HB2	1.95	0.65
1:A:2100:LEU:C	1:A:2103:GLN:HG3	2.20	0.65
1:B:2219:TYR:CD1	1:B:2223:TRP:HD1	2.15	0.64
1:A:2166:PRO:HG2	2:C:269:TRP:CE3	2.30	0.63
1:B:2224:GLY:N	1:B:2225:PRO:HD2	2.14	0.62
1:B:2109:TRP:CD1	1:B:2204:SER:HG	2.17	0.62
1:B:2292:LEU:HD23	1:B:2292:LEU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2195:GLN:C	1:B:2197:PRO:HD2	2.25	0.62
1:A:2178:GLN:NE2	1:A:2237:ASN:OD1	2.28	0.62
1:A:2126:ASP:OD1	1:A:2126:ASP:N	2.30	0.61
1:A:2236:ASN:O	1:A:2237:ASN:HB2	1.99	0.61
1:B:2294:ASN:O	1:B:2295:ASN:HB2	2.00	0.61
1:B:2133:THR:C	1:B:2152:VAL:HG12	2.26	0.60
1:A:2264:SER:HA	1:A:2292:LEU:HB3	1.82	0.60
1:A:2241:LEU:HB2	1:A:2254:ILE:CG2	2.31	0.59
1:A:2273:ASN:HD21	1:A:2278:THR:H	1.49	0.59
1:A:2100:LEU:O	1:A:2103:GLN:CG	2.46	0.59
1:A:2160:LEU:HB2	1:A:2173:HIS:CE1	2.36	0.59
1:B:2113:GLU:CD	1:B:2115:SER:OG	2.46	0.59
1:A:2225:PRO:O	1:A:2228:ASN:N	2.29	0.58
1:A:2105:SER:CB	1:B:2114:TRP:HE1	2.04	0.58
1:B:2196:LEU:N	1:B:2197:PRO:CD	2.66	0.58
1:A:2105:SER:O	1:B:2147:ARG:NH1	2.37	0.57
1:B:2109:TRP:HD1	1:B:2204:SER:OG	1.88	0.57
1:B:2219:TYR:CE1	1:B:2223:TRP:CD1	2.93	0.57
1:A:2147:ARG:HA	1:A:2194:HIS:HB2	1.87	0.57
1:B:2114:TRP:O	1:B:2114:TRP:CD1	2.58	0.57
1:A:2287:LEU:HD23	1:A:2300:VAL:CG2	2.35	0.56
1:A:2141:PHE:N	1:A:2142:PRO:CD	2.68	0.56
1:A:2157:GLN:HG2	4:A:2530:HOH:O	2.05	0.56
1:A:2262:TYR:HA	4:A:2507:HOH:O	2.04	0.56
2:C:268:LYS:HG3	2:C:269:TRP:H	1.71	0.56
1:B:2113:GLU:CD	1:B:2115:SER:HG	2.14	0.55
1:B:2132:ILE:CG2	1:B:2151:ILE:HG23	2.36	0.55
1:B:2219:TYR:CE1	1:B:2223:TRP:HD1	2.25	0.55
1:A:2132:ILE:HG13	1:A:2196:LEU:HD11	1.88	0.55
1:B:2133:THR:CG2	1:B:2152:VAL:HG11	2.36	0.55
1:B:2161:ASP:OD2	1:B:2164:GLN:HG2	2.07	0.55
1:A:2286:ILE:HG23	1:A:2303:GLN:CG	2.35	0.55
1:B:2224:GLY:N	1:B:2225:PRO:CD	2.70	0.55
1:B:2257:PHE:HB2	1:B:2268:PRO:HB2	1.89	0.55
1:A:2102:ASP:O	1:B:2147:ARG:NH1	2.40	0.54
1:A:2287:LEU:CD2	1:A:2300:VAL:HG21	2.38	0.54
1:B:2235:ASN:O	1:B:2238:GLU:HB2	2.08	0.54
2:C:266:GLN:OE1	2:C:269:TRP:HD1	1.90	0.54
1:B:2239:LEU:CD1	1:B:2258:LEU:HD11	2.38	0.54
1:B:2239:LEU:HD11	1:B:2258:LEU:HD11	1.90	0.54
1:A:2239:LEU:HD22	1:A:2258:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2100:LEU:CA	1:A:2103:GLN:CG	2.85	0.53
1:B:2246:SER:N	4:B:2411:HOH:O	2.22	0.53
1:A:2294:ASN:N	1:A:2294:ASN:OD1	2.42	0.52
1:B:2306:GLN:HA	1:B:2310:GLN:HB2	1.91	0.52
1:A:2227:TYR:CE1	1:A:2302:LYS:CG	2.91	0.52
1:B:2237:ASN:O	1:B:2237:ASN:OD1	2.28	0.52
1:B:2109:TRP:HD1	1:B:2204:SER:HG	1.54	0.52
1:A:2096:ARG:O	1:A:2100:LEU:HG	2.09	0.51
1:A:2309:PHE:N	1:A:2309:PHE:CD2	2.76	0.51
1:B:2168:SER:O	1:B:2172:VAL:HG23	2.10	0.51
1:B:2213:LEU:HD21	1:B:2258:LEU:HD13	1.93	0.51
1:B:2240:ARG:HH11	1:B:2240:ARG:HG2	1.76	0.51
1:B:2229:LEU:CD1	1:B:2241:LEU:HB3	2.40	0.50
1:A:2222:ARG:NH1	1:A:2223:TRP:CH2	2.79	0.50
1:B:2245:SER:CB	1:B:2309:PHE:CD1	2.95	0.50
1:B:2133:THR:O	1:B:2152:VAL:CG1	2.58	0.50
1:B:2113:GLU:OE2	1:B:2115:SER:OG	2.30	0.49
1:A:2235:ASN:O	1:A:2238:GLU:HB2	2.13	0.49
1:A:2135:GLU:HA	1:A:2152:VAL:CG2	2.42	0.49
1:A:2219:TYR:CE2	1:A:2298:LYS:HD2	2.48	0.49
1:B:2113:GLU:OE1	1:B:2115:SER:OG	2.30	0.49
1:A:2100:LEU:CA	1:A:2103:GLN:HG3	2.43	0.49
1:B:2177:PHE:HD1	1:B:2177:PHE:O	1.95	0.49
2:C:267:ARG:O	2:C:268:LYS:C	2.54	0.49
1:B:2255:THR:O	1:B:2269:SER:HA	2.12	0.49
1:B:2294:ASN:O	1:B:2295:ASN:CB	2.60	0.48
1:A:2123:PHE:HB2	1:A:2128:ILE:HB	1.95	0.48
1:A:2308:LEU:C	1:A:2309:PHE:CD2	2.91	0.48
1:A:2175:LEU:CD2	1:A:2237:ASN:HD21	2.27	0.47
1:B:2187:LYS:HG3	1:B:2188:LYS:N	2.29	0.47
1:A:2229:LEU:HD21	1:A:2232:ILE:HD11	1.96	0.47
1:A:2308:LEU:HB2	1:A:2309:PHE:CD2	2.49	0.47
1:A:2099:GLU:O	1:A:2102:ASP:CB	2.59	0.47
1:A:2255:THR:O	1:A:2269:SER:HA	2.15	0.47
1:A:2297:LEU:O	1:A:2300:VAL:HG12	2.15	0.47
1:B:2153:ASP:CG	1:B:2154:VAL:N	2.72	0.47
1:A:2175:LEU:HD21	1:A:2237:ASN:ND2	2.30	0.47
1:B:2133:THR:CG2	1:B:2152:VAL:CG1	2.90	0.47
1:A:2251:LYS:HE2	1:A:2274:HIS:ND1	2.29	0.47
1:A:2198:LYS:O	1:A:2202:GLU:HG3	2.15	0.47
1:A:2168:SER:O	1:A:2172:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:268:LYS:HG3	2:C:269:TRP:N	2.30	0.46
1:A:2106:LEU:HD23	1:A:2106:LEU:HA	1.76	0.46
1:B:2233:ASP:HB3	1:B:2240:ARG:HB2	1.98	0.46
1:B:2220:LEU:HA	1:B:2220:LEU:HD23	1.59	0.45
1:B:2135:GLU:HB3	4:B:2408:HOH:O	2.16	0.45
1:B:2167:PRO:HB2	1:B:2234:ILE:HD12	1.98	0.45
1:B:2240:ARG:HG2	1:B:2240:ARG:NH1	2.31	0.45
1:A:2222:ARG:HD3	1:A:2223:TRP:CZ2	2.51	0.45
1:A:2197:PRO:HG3	1:B:2141:PHE:CD2	2.52	0.45
1:B:2232:ILE:HG22	1:B:2233:ASP:N	2.32	0.45
1:B:2132:ILE:HG22	1:B:2151:ILE:HG23	2.00	0.44
1:A:2297:LEU:HA	1:A:2297:LEU:HD12	1.77	0.44
1:B:2307:ASP:CB	1:B:2308:LEU:HD13	2.47	0.44
1:A:2264:SER:O	1:A:2292:LEU:CD1	2.46	0.44
1:B:2109:TRP:HB3	1:B:2123:PHE:CD1	2.49	0.44
1:A:2273:ASN:HD21	1:A:2278:THR:N	2.13	0.44
1:A:2224:GLY:N	1:A:2225:PRO:CD	2.80	0.44
1:A:2127:THR:O	1:A:2159:LEU:N	2.41	0.44
1:A:2100:LEU:C	1:A:2103:GLN:CG	2.89	0.44
1:A:2153:ASP:HB3	4:A:2528:HOH:O	2.17	0.44
1:A:2100:LEU:HA	1:A:2103:GLN:HG3	1.93	0.44
1:A:2262:TYR:CG	1:A:2263:PRO:HA	2.52	0.44
1:B:2289:LYS:HD2	1:B:2303:GLN:HE21	1.83	0.44
1:A:2262:TYR:CG	1:A:2263:PRO:CA	3.01	0.43
1:A:2135:GLU:N	1:A:2152:VAL:HG23	2.34	0.43
1:B:2184:GLU:HB3	1:B:2187:LYS:HE2	2.00	0.43
1:A:2162:GLU:HG2	1:A:2170:LEU:CD2	2.49	0.43
1:B:2132:ILE:HG23	1:B:2151:ILE:CG2	2.49	0.43
1:B:2237:ASN:OD1	1:B:2237:ASN:C	2.61	0.43
1:A:2309:PHE:N	1:A:2309:PHE:HD2	2.17	0.43
1:A:2254:ILE:CD1	1:A:2283:ILE:HG21	2.49	0.43
1:A:2308:LEU:N	1:A:2308:LEU:CD2	2.40	0.42
1:B:2226:ASN:OD1	1:B:2226:ASN:N	2.52	0.42
1:A:2243:PHE:O	1:A:2251:LYS:HA	2.19	0.42
1:A:2124:VAL:O	1:A:2124:VAL:HG12	2.20	0.42
1:A:2147:ARG:HB2	1:A:2147:ARG:CZ	2.50	0.42
1:B:2112:VAL:HG21	1:B:2122:THR:HG23	2.02	0.42
1:A:2219:TYR:CD2	1:A:2298:LYS:HD2	2.55	0.42
1:B:2289:LYS:HD2	1:B:2303:GLN:NE2	2.35	0.42
1:A:2175:LEU:CD2	1:A:2237:ASN:ND2	2.84	0.41
1:A:2224:GLY:N	1:A:2225:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2116:ASP:CG	1:B:2117:ASP:N	2.72	0.41
1:A:2239:LEU:HD12	1:A:2239:LEU:HA	1.92	0.41
1:B:2132:ILE:CG2	1:B:2151:ILE:CG2	2.98	0.41
1:B:2229:LEU:HD11	1:B:2241:LEU:HB3	2.03	0.41
1:B:2307:ASP:HB3	1:B:2308:LEU:CD1	2.50	0.41
1:B:2114:TRP:O	1:B:2114:TRP:CG	2.72	0.41
1:B:2156:PHE:C	1:B:2157:GLN:HG3	2.45	0.41
1:B:2292:LEU:N	1:B:2292:LEU:CD2	2.81	0.41
1:A:2256:LEU:HD23	1:A:2269:SER:HB3	2.03	0.41
1:B:2122:THR:HG22	1:B:2129:GLN:HG2	2.02	0.41
1:A:2159:LEU:HG	2:C:273:ARG:NH2	2.36	0.40
1:A:2262:TYR:CE1	1:A:2296:TYR:HB3	2.55	0.40
1:A:2124:VAL:C	1:A:2125:TYR:CD2	2.99	0.40
1:A:2262:TYR:HE1	1:A:2296:TYR:HB3	1.85	0.40
1:A:2225:PRO:C	1:A:2227:TYR:N	2.79	0.40
1:A:2290:VAL:CG1	1:A:2296:TYR:HD1	2.35	0.40
1:B:2222:ARG:HG3	1:B:2223:TRP:CE2	2.56	0.40
1:B:2224:GLY:O	1:B:2227:TYR:N	2.40	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	214/221 (97%)	202 (94%)	12 (6%)	0	100	100
1	B	205/221 (93%)	193 (94%)	12 (6%)	0	100	100
2	C	7/26 (27%)	5 (71%)	2 (29%)	0	100	100
2	D	7/26 (27%)	7 (100%)	0	0	100	100
All	All	433/494 (88%)	407 (94%)	26 (6%)	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	205/208 (99%)	195 (95%)	10 (5%)	22	55
1	B	196/208 (94%)	183 (93%)	13 (7%)	15	43
2	C	9/26 (35%)	8 (89%)	1 (11%)	6	20
2	D	9/26 (35%)	9 (100%)	0	100	100
All	All	419/468 (90%)	395 (94%)	24 (6%)	18	49

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

Mol	Chain	Res	Type
1	A	2096	ARG
1	A	2103	GLN
1	A	2112	VAL
1	A	2126	ASP
1	A	2237	ASN
1	A	2254	ILE
1	A	2293	GLU
1	A	2294	ASN
1	A	2308	LEU
1	A	2310	GLN
1	B	2113	GLU
1	B	2128	ILE
1	B	2130	LEU
1	B	2142	PRO
1	B	2157	GLN
1	B	2170	LEU
1	B	2185	SER
1	B	2225	PRO
1	B	2232	ILE
1	B	2237	ASN
1	B	2292	LEU
1	B	2308	LEU
1	B	2310	GLN
2	C	273	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2273	ASN
1	A	2303	GLN
1	B	2155	ASN
1	B	2157	GLN
1	B	2178	GLN
1	B	2195	GLN
1	B	2237	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	214/221 (96%)	0.01	8 (3%)	45	36	28, 49, 88, 133	0
1	B	205/221 (92%)	0.27	9 (4%)	39	31	35, 61, 96, 115	0
2	C	9/26 (34%)	0.85	0	100	100	36, 68, 79, 84	0
2	D	9/26 (34%)	0.80	0	100	100	61, 88, 103, 108	0
All	All	437/494 (88%)	0.17	17 (3%)	43	34	28, 56, 94, 133	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2294	ASN	5.0
1	A	2100	LEU	4.0
1	A	2104	LEU	3.8
1	A	2263	PRO	3.8
1	B	2106	LEU	3.4
1	B	2114	TRP	3.3
1	B	2105	SER	3.2
1	A	2103	GLN	3.0
1	B	2107	SER	3.0
1	A	2097	THR	2.9
1	A	2102	ASP	2.8
1	B	2194	HIS	2.7
1	A	2264	SER	2.3
1	B	2292	LEU	2.2
1	A	2101	LEU	2.2
1	B	2112	VAL	2.1
1	B	2163	ASP	2.0

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

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](#)

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($\text{\AA}^2$)	Q<0.9
3	CL	A	2401	1/1	0.94	0.06	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.