



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:49 AM UTC

PDB ID : 5F6H / pdb_00005f6h
Title : Crystal Structure of Tier 2 Neutralizing Antibody DH427 from a Rhesus Macaque
Authors : Fera, D.; Harrison, S.C.
Deposited on : 2015-12-06
Resolution : 2.66 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

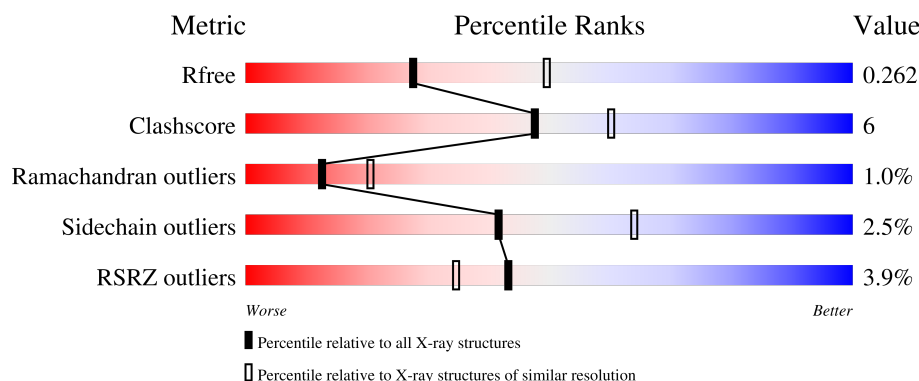
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	J	216	 7% 85% 12% ..
1	L	216	 2% 83% 14% .
1	N	216	 7% 83% 15% .
1	P	216	 4% 83% 15% .
2	I	227	 2% 78% 14% . 7%

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Mol	Chain	Length	Quality of chain
2	K	227	3% 77% 15% 7%
2	M	227	3% 79% 13% 7%
2	O	227	2% 77% 14% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12691 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 DH427 Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1574	979	264	326	5			
1	J	212	Total	C	N	O	S	0	0	0
			1574	979	264	326	5			
1	N	212	Total	C	N	O	S	0	0	0
			1574	979	264	326	5			
1	P	212	Total	C	N	O	S	0	0	0
			1574	979	264	326	5			

- Molecule 2 is a protein called DH427 Antibody Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	210	Total	C	N	O	S	0	0	0
			1572	996	262	307	7			
2	I	210	Total	C	N	O	S	0	0	0
			1572	996	262	307	7			
2	M	210	Total	C	N	O	S	0	0	0
			1572	996	262	307	7			
2	O	210	Total	C	N	O	S	0	0	0
			1572	996	262	307	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	3	Total	O	0	0
			3	3		
3	J	14	Total	O	0	0
			14	14		
3	N	17	Total	O	0	0
			17	17		
3	P	17	Total	O	0	0
			17	17		

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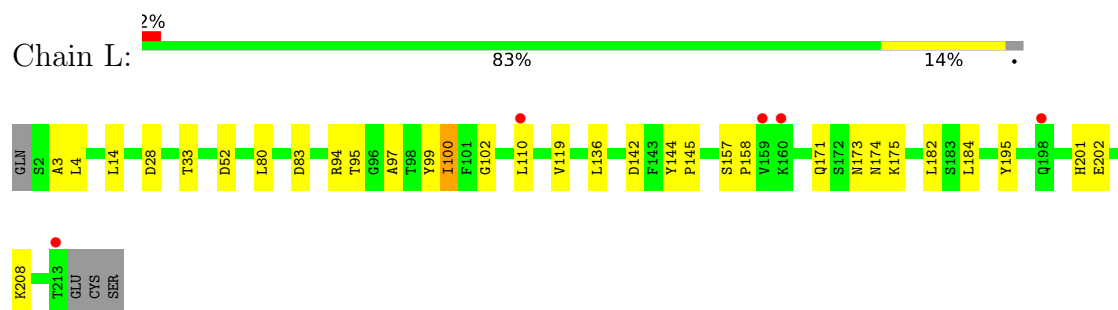
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	11	Total 11	O 11	0	0
3	M	23	Total 23	O 23	0	0
3	O	22	Total 22	O 22	0	0

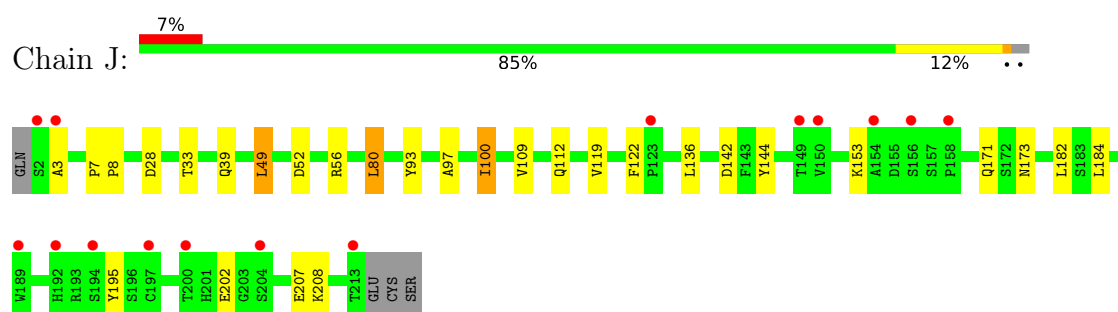
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

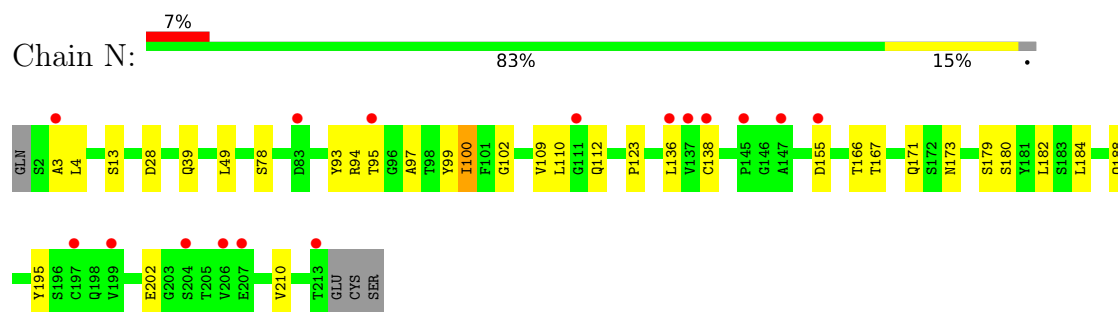
- Molecule 1: DH427 Antibody Light Chain



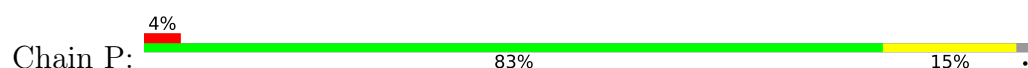
- Molecule 1: DH427 Antibody Light Chain

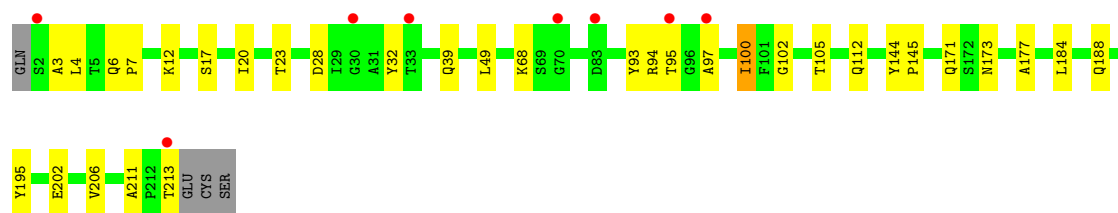


- Molecule 1: DH427 Antibody Light Chain

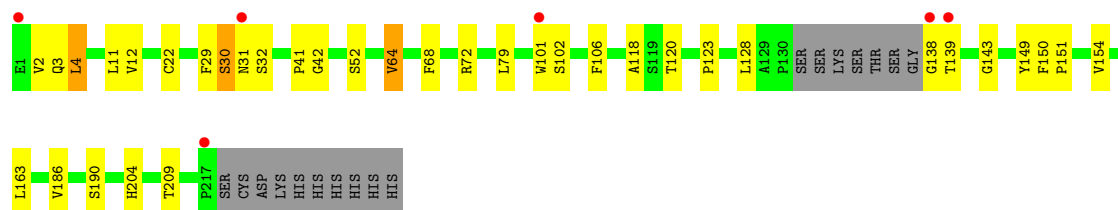
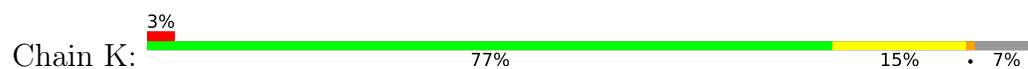


- Molecule 1: DH427 Antibody Light Chain

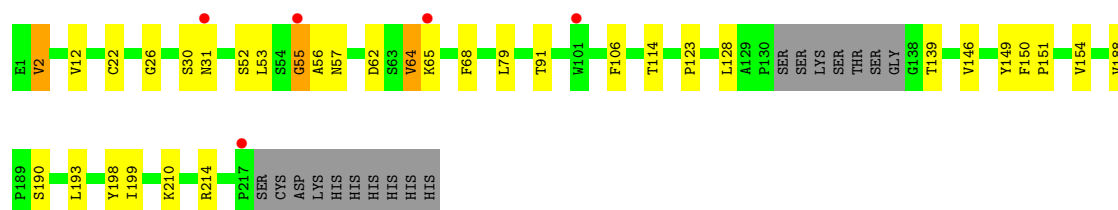
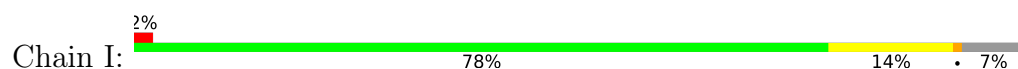




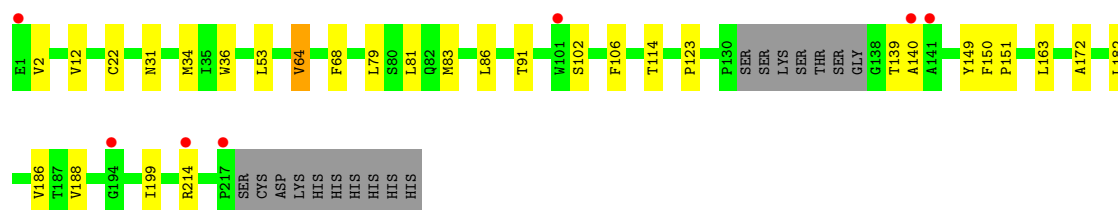
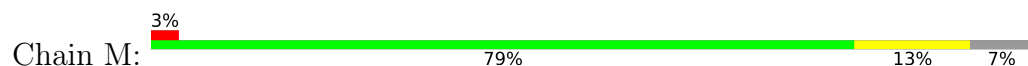
• Molecule 2: DH427 Antibody Heavy Chain



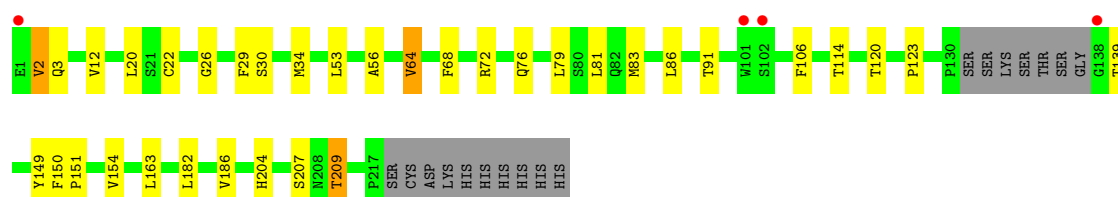
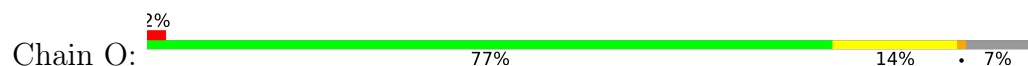
• Molecule 2: DH427 Antibody Heavy Chain



• Molecule 2: DH427 Antibody Heavy Chain



• Molecule 2: DH427 Antibody Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.88Å 153.79Å 162.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.66 48.90 – 2.66	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.90-2.66) 89.7 (48.90-2.66)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.48 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.230 , 0.262 0.228 , 0.262	Depositor DCC
R_{free} test set	2861 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12691	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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 [i](#)

5.1 Standard geometry [i](#)

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	J	0.29	0/1610	0.72	0/2198
1	L	0.29	0/1610	0.74	0/2198
1	N	0.29	0/1610	0.76	2/2198 (0.1%)
1	P	0.30	0/1610	0.73	0/2198
2	I	0.30	0/1610	0.76	1/2193 (0.0%)
2	K	0.30	0/1610	0.77	1/2193 (0.0%)
2	M	0.29	0/1610	0.75	0/2193
2	O	0.31	0/1610	0.74	0/2193
All	All	0.30	0/12880	0.75	4/17564 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	55	GLY	N-CA-C	-8.51	100.98	111.45
1	N	167	THR	CA-C-N	5.78	125.74	119.78
1	N	167	THR	C-N-CA	5.78	125.74	119.78
2	K	143	GLY	N-CA-C	5.32	118.91	111.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	J	1574	0	1525	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1574	0	1525	20	0
1	N	1574	0	1525	22	0
1	P	1574	0	1525	20	0
2	I	1572	0	1530	16	0
2	K	1572	0	1530	17	0
2	M	1572	0	1530	14	0
2	O	1572	0	1530	18	0
3	I	11	0	0	0	0
3	J	14	0	0	0	0
3	L	3	0	0	0	0
3	M	23	0	0	0	1
3	N	17	0	0	2	0
3	O	22	0	0	0	1
3	P	17	0	0	0	0
All	All	12691	0	12220	139	1

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 (139) 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)
2:I:199:ILE:HG12	2:I:214:ARG:HG2	1.54	0.90
2:K:30:SER:O	2:K:32:SER:N	2.08	0.86
1:N:3:ALA:HA	1:N:100:ILE:HD11	1.61	0.81
1:J:3:ALA:HA	1:J:100:ILE:HD11	1.64	0.78
2:M:199:ILE:HG12	2:M:214:ARG:HG2	1.68	0.75
1:N:123:PRO:HB3	1:N:210:VAL:HG11	1.70	0.73
2:I:62:ASP:HA	2:I:65:LYS:HE3	1.73	0.71
2:O:204:HIS:HB3	2:O:209:THR:HG23	1.74	0.70
2:I:22:CYS:HB3	2:I:79:LEU:HB3	1.75	0.69
1:L:119:VAL:O	1:L:208:LYS:NZ	2.25	0.68
2:I:52:SER:OG	2:I:55:GLY:O	2.11	0.67
1:P:6:GLN:HE21	1:P:105:THR:HG23	1.59	0.66
1:P:7:PRO:O	1:P:105:THR:HG22	1.97	0.64
2:M:140:ALA:N	2:M:188:VAL:O	2.27	0.63
1:L:136:LEU:HD22	1:L:182:LEU:HD23	1.80	0.63
1:J:182:LEU:HG	1:J:184:LEU:HD13	1.81	0.62
1:N:94:ARG:HG2	1:N:95:THR:HG23	1.80	0.62
1:J:39:GLN:HB2	1:J:49:LEU:HD21	1.82	0.62
2:M:64:VAL:HG13	2:M:68:PHE:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:64:VAL:HG13	2:K:68:PHE:HB2	1.82	0.60
1:N:93:TYR:CE1	1:N:97:ALA:HA	2.36	0.60
1:N:166:THR:HG22	1:N:179:SER:H	1.66	0.60
1:N:136:LEU:HB2	1:N:182:LEU:HB3	1.83	0.59
2:K:30:SER:C	2:K:32:SER:H	2.12	0.58
2:O:163:LEU:HD21	2:O:186:VAL:HG21	1.86	0.58
1:L:182:LEU:HG	1:L:184:LEU:HD13	1.84	0.57
1:J:153:LYS:HZ1	1:J:207:GLU:CD	2.13	0.57
1:P:20:ILE:HG23	1:P:105:THR:HG21	1.86	0.56
1:P:6:GLN:NE2	1:P:105:THR:HG23	2.20	0.56
2:K:138:GLY:N	1:N:78:SER:HG	2.04	0.55
2:K:22:CYS:HB3	2:K:79:LEU:HB3	1.88	0.54
2:I:64:VAL:HG13	2:I:68:PHE:HB2	1.89	0.54
2:I:190:SER:HA	2:I:193:LEU:HD13	1.87	0.54
1:J:93:TYR:CE1	1:J:97:ALA:HA	2.42	0.54
2:O:64:VAL:HG13	2:O:68:PHE:HB2	1.90	0.53
1:J:119:VAL:O	1:J:208:LYS:NZ	2.37	0.53
2:M:163:LEU:HD21	2:M:186:VAL:HG21	1.91	0.53
1:L:3:ALA:HA	1:L:100:ILE:HD11	1.91	0.53
1:J:142:ASP:OD1	1:J:173:ASN:ND2	2.42	0.53
2:I:146:VAL:HG11	2:I:154:VAL:HG11	1.90	0.53
2:K:123:PRO:HB3	2:K:149:TYR:HB3	1.91	0.52
2:M:31:ASN:HA	2:M:53:LEU:HD22	1.92	0.52
1:L:94:ARG:HG2	1:L:95:THR:H	1.73	0.52
1:L:142:ASP:OD1	1:L:173:ASN:ND2	2.42	0.52
2:M:91:THR:HG23	2:M:114:THR:HA	1.92	0.51
2:K:29:PHE:O	2:K:72:ARG:NH2	2.43	0.51
1:J:136:LEU:HD22	1:J:182:LEU:HD23	1.92	0.51
1:P:39:GLN:HB2	1:P:49:LEU:HD11	1.91	0.51
1:P:94:ARG:HG2	1:P:95:THR:H	1.75	0.51
2:I:55:GLY:O	2:I:57:ASN:N	2.35	0.51
1:L:136:LEU:HB2	1:L:182:LEU:HB3	1.92	0.51
2:M:83:MET:HB3	2:M:86:LEU:HD21	1.92	0.51
1:P:93:TYR:CE1	1:P:97:ALA:HA	2.46	0.50
1:N:109:VAL:O	1:N:112:GLN:NE2	2.40	0.49
2:I:62:ASP:O	2:I:65:LYS:HG2	2.13	0.49
1:N:97:ALA:O	3:N:301:HOH:O	2.20	0.49
2:I:31:ASN:HA	2:I:53:LEU:HD22	1.94	0.49
2:K:52:SER:O	2:K:72:ARG:NH1	2.45	0.49
2:K:163:LEU:HD21	2:K:186:VAL:HG21	1.95	0.49
1:N:4:LEU:HB2	1:N:102:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:91:THR:HG23	2:I:114:THR:HA	1.94	0.48
2:M:22:CYS:HB3	2:M:79:LEU:HB3	1.95	0.48
1:J:112:GLN:HB2	1:J:144:TYR:CE2	2.48	0.48
2:O:30:SER:O	2:O:53:LEU:HB2	2.13	0.48
2:O:123:PRO:HB3	2:O:149:TYR:HB3	1.95	0.48
1:N:184:LEU:HD11	1:N:195:TYR:CZ	2.49	0.48
1:J:184:LEU:HD21	1:J:195:TYR:CE1	2.48	0.47
1:N:136:LEU:HD22	1:N:182:LEU:HD23	1.95	0.47
1:P:12:LYS:HD2	1:P:17:SER:O	2.14	0.47
1:L:171:GLN:HB2	1:L:173:ASN:OD1	2.15	0.47
1:J:33:THR:O	1:J:52:ASP:HA	2.15	0.47
1:L:184:LEU:HD21	1:L:195:TYR:CZ	2.50	0.46
2:K:204:HIS:HB3	2:K:209:THR:HB	1.96	0.46
1:J:122:PHE:CD1	2:I:128:LEU:HB3	2.51	0.46
2:O:150:PHE:HA	2:O:151:PRO:HA	1.74	0.46
1:J:171:GLN:HB2	1:J:173:ASN:OD1	2.15	0.46
1:P:112:GLN:HB2	1:P:144:TYR:CE2	2.50	0.46
2:M:123:PRO:HB3	2:M:149:TYR:HB3	1.96	0.46
1:L:95:THR:C	1:L:97:ALA:H	2.24	0.46
1:N:138:CYS:HB3	1:N:180:SER:HB3	1.97	0.46
1:J:109:VAL:O	1:J:112:GLN:NE2	2.43	0.46
1:P:171:GLN:OE1	1:P:177:ALA:HB2	2.16	0.46
2:M:34:MET:HB3	2:M:79:LEU:HD22	1.99	0.45
2:O:83:MET:HB3	2:O:86:LEU:HD21	1.97	0.45
1:L:14:LEU:HB3	1:P:206:VAL:HG12	1.97	0.45
1:N:39:GLN:HB2	1:N:49:LEU:HD11	1.96	0.45
1:N:171:GLN:HB2	1:N:173:ASN:OD1	2.16	0.45
2:O:29:PHE:CE1	2:O:34:MET:HE3	2.51	0.45
2:O:2:VAL:HA	2:O:26:GLY:HA3	1.99	0.45
2:O:22:CYS:HB3	2:O:79:LEU:HB3	1.98	0.45
1:N:184:LEU:HD11	1:N:195:TYR:CE1	2.52	0.45
2:O:123:PRO:HD2	2:O:209:THR:HG21	1.97	0.45
1:L:4:LEU:HB2	1:L:102:GLY:HA2	1.99	0.45
2:I:123:PRO:HB3	2:I:149:TYR:HB3	1.98	0.45
2:I:188:VAL:HG11	2:I:198:TYR:CE1	2.52	0.45
1:J:136:LEU:HB2	1:J:182:LEU:HB3	1.99	0.44
2:K:150:PHE:HA	2:K:151:PRO:HA	1.81	0.44
1:N:93:TYR:CZ	1:N:97:ALA:HA	2.53	0.44
1:L:145:PRO:O	1:L:201:HIS:HE1	2.00	0.44
1:N:95:THR:HA	3:N:317:HOH:O	2.18	0.44
1:N:184:LEU:HD22	1:N:188:GLN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:3:ALA:HA	1:P:100:ILE:HD11	1.99	0.44
1:N:99:TYR:OH	2:M:102:SER:HA	2.18	0.43
1:L:99:TYR:OH	2:K:102:SER:HA	2.18	0.43
2:K:11:LEU:HD23	2:K:120:THR:HG23	2.00	0.43
2:O:154:VAL:HG23	2:O:182:LEU:HD21	2.01	0.43
2:K:3:GLN:O	2:K:4:LEU:HD13	2.18	0.43
2:K:11:LEU:HD21	2:K:118:ALA:O	2.19	0.43
2:M:36:TRP:CE2	2:M:81:LEU:HB2	2.54	0.43
1:N:95:THR:C	1:N:97:ALA:H	2.27	0.43
1:P:171:GLN:NE2	1:P:173:ASN:OD1	2.42	0.43
1:P:211:ALA:C	1:P:213:THR:H	2.26	0.43
2:O:20:LEU:HD12	2:O:81:LEU:HD23	1.99	0.43
1:L:157:SER:HA	1:L:158:PRO:HD3	1.93	0.43
2:O:29:PHE:O	2:O:72:ARG:NH2	2.52	0.43
1:L:144:TYR:CG	1:L:145:PRO:HA	2.54	0.42
2:I:150:PHE:HA	2:I:151:PRO:HA	1.77	0.42
1:P:184:LEU:HD11	1:P:195:TYR:CZ	2.54	0.42
1:N:13:SER:HA	1:N:110:LEU:HB2	2.01	0.42
1:P:4:LEU:HB2	1:P:102:GLY:HA2	2.01	0.42
2:M:172:ALA:HA	2:M:182:LEU:HB3	2.00	0.42
2:O:120:THR:CG2	2:O:207:SER:HB3	2.50	0.41
2:K:30:SER:C	2:K:32:SER:N	2.76	0.41
1:P:32:TYR:O	1:P:68:LYS:NZ	2.54	0.41
1:L:83:ASP:OD1	1:L:174:ASN:ND2	2.49	0.41
2:K:41:PRO:HA	2:K:42:GLY:HA2	1.67	0.41
2:M:150:PHE:HA	2:M:151:PRO:HA	1.80	0.41
1:P:184:LEU:HD22	1:P:188:GLN:HB3	2.03	0.41
1:L:142:ASP:H	1:L:171:GLN:HE22	1.67	0.41
1:J:7:PRO:HA	1:J:8:PRO:HD3	1.94	0.41
1:P:144:TYR:CG	1:P:145:PRO:HA	2.55	0.41
1:L:110:LEU:HD23	1:L:110:LEU:HA	1.93	0.41
2:O:29:PHE:CD1	2:O:34:MET:HE3	2.56	0.41
1:J:80:LEU:HD12	1:J:80:LEU:HA	1.85	0.40
2:I:2:VAL:HA	2:I:26:GLY:HA3	2.04	0.40
1:L:33:THR:O	1:L:52:ASP:HA	2.22	0.40
1:P:6:GLN:HB3	1:P:105:THR:CG2	2.52	0.40
2:O:34:MET:HB3	2:O:79:LEU:HD22	2.02	0.40
2:O:91:THR:HG23	2:O:114:THR:HA	2.02	0.40

All (1) 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)
3:M:302:HOH:O	3:O:314:HOH:O[1_655]	2.12	0.08

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	J	210/216 (97%)	200 (95%)	9 (4%)	1 (0%)	24	39
1	L	210/216 (97%)	201 (96%)	8 (4%)	1 (0%)	24	39
1	N	210/216 (97%)	196 (93%)	12 (6%)	2 (1%)	12	20
1	P	210/216 (97%)	200 (95%)	9 (4%)	1 (0%)	24	39
2	I	206/227 (91%)	196 (95%)	7 (3%)	3 (2%)	8	13
2	K	206/227 (91%)	193 (94%)	9 (4%)	4 (2%)	6	10
2	M	206/227 (91%)	196 (95%)	8 (4%)	2 (1%)	12	20
2	O	206/227 (91%)	194 (94%)	9 (4%)	3 (2%)	8	13
All	All	1664/1772 (94%)	1576 (95%)	71 (4%)	17 (1%)	12	20

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	30	SER
2	K	31	ASN
2	K	139	THR
2	I	139	THR
2	O	139	THR
2	M	106	PHE
2	M	139	THR
2	O	106	PHE
2	K	106	PHE
1	J	202	GLU
2	I	106	PHE
1	P	202	GLU

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Mol	Chain	Res	Type
2	O	56	ALA
1	L	202	GLU
1	N	155	ASP
1	N	202	GLU
2	I	56	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	J	179/183 (98%)	174 (97%)	5 (3%)	38	60
1	L	179/183 (98%)	175 (98%)	4 (2%)	45	67
1	N	179/183 (98%)	177 (99%)	2 (1%)	65	80
1	P	179/183 (98%)	176 (98%)	3 (2%)	53	73
2	I	175/191 (92%)	170 (97%)	5 (3%)	37	58
2	K	175/191 (92%)	167 (95%)	8 (5%)	24	41
2	M	175/191 (92%)	172 (98%)	3 (2%)	53	73
2	O	175/191 (92%)	169 (97%)	6 (3%)	32	53
All	All	1416/1496 (95%)	1380 (98%)	36 (2%)	42	64

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	28	ASP
1	L	80	LEU
1	L	100	ILE
1	L	175	LYS
2	K	2	VAL
2	K	4	LEU
2	K	12	VAL
2	K	64	VAL
2	K	101	TRP
2	K	128	LEU

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Mol	Chain	Res	Type
2	K	154	VAL
2	K	190	SER
1	J	28	ASP
1	J	49	LEU
1	J	56	ARG
1	J	80	LEU
1	J	100	ILE
1	N	28	ASP
1	N	100	ILE
1	P	23	THR
1	P	28	ASP
1	P	100	ILE
2	I	2	VAL
2	I	12	VAL
2	I	30	SER
2	I	64	VAL
2	I	210	LYS
2	M	2	VAL
2	M	12	VAL
2	M	64	VAL
2	O	2	VAL
2	O	3	GLN
2	O	12	VAL
2	O	64	VAL
2	O	76	GLN
2	O	209	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	76	GLN
2	K	208	ASN
1	J	198	GLN
1	P	39	GLN
2	M	84	ASN
2	M	196	GLN
2	O	3	GLN
2	O	76	GLN
2	O	168	HIS
2	O	196	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 [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	J	212/216 (98%)	0.46	15 (7%)	22	16	10, 34, 70, 85	0
1	L	212/216 (98%)	0.17	5 (2%)	59	53	10, 24, 57, 77	0
1	N	212/216 (98%)	0.53	16 (7%)	20	15	9, 37, 64, 78	0
1	P	212/216 (98%)	0.19	8 (3%)	44	36	9, 28, 49, 61	0
2	I	210/227 (92%)	-0.01	5 (2%)	59	53	9, 17, 52, 65	0
2	K	210/227 (92%)	-0.04	6 (2%)	53	46	9, 16, 46, 64	0
2	M	210/227 (92%)	0.02	7 (3%)	49	40	10, 18, 55, 71	0
2	O	210/227 (92%)	0.10	4 (1%)	66	61	11, 20, 44, 73	0
All	All	1688/1772 (95%)	0.18	66 (3%)	43	35	9, 22, 59, 85	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	138	GLY	6.5
1	N	206	VAL	4.0
1	P	213	THR	4.0
2	O	101	TRP	3.6
2	I	55	GLY	3.6
2	I	65	LYS	3.4
2	M	1	GLU	3.3
2	K	138	GLY	3.2
1	N	199	VAL	3.2
1	J	213	THR	3.2
1	N	213	THR	3.2
1	N	207	GLU	3.1
1	J	2	SER	3.0
1	J	3	ALA	3.0
2	K	101	TRP	3.0
1	P	95	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	197	CYS	2.9
1	P	97	ALA	2.9
2	K	139	THR	2.8
1	L	213	THR	2.8
1	P	83	ASP	2.8
2	I	101	TRP	2.7
1	J	154	ALA	2.7
1	J	204	SER	2.7
1	N	204	SER	2.7
1	J	200	THR	2.7
2	I	217	PRO	2.6
1	N	155	ASP	2.6
1	J	197	CYS	2.6
1	L	160	LYS	2.6
2	M	140	ALA	2.5
2	M	101	TRP	2.5
1	J	149	THR	2.4
1	N	145	PRO	2.4
1	N	3	ALA	2.4
2	M	217	PRO	2.4
1	N	138	CYS	2.4
1	L	159	VAL	2.4
1	P	2	SER	2.4
1	N	147	ALA	2.3
2	I	31	ASN	2.3
1	J	158	PRO	2.3
1	J	156	SER	2.3
2	O	1	GLU	2.2
1	J	194	SER	2.2
2	M	141	ALA	2.2
1	L	198	GLN	2.2
2	M	214	ARG	2.2
1	J	192	HIS	2.2
1	N	111	GLY	2.2
2	M	194	GLY	2.2
1	N	137	VAL	2.2
1	N	83	ASP	2.1
1	J	189	TRP	2.1
2	K	1	GLU	2.1
2	K	217	PRO	2.1
1	J	123	PRO	2.1
2	K	31	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	33	THR	2.1
2	O	102	SER	2.0
1	N	95	THR	2.0
1	P	70	GLY	2.0
1	L	110	LEU	2.0
1	N	136	LEU	2.0
1	P	30	GLY	2.0
1	J	150	VAL	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.