



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:16 pm BST

PDB ID : 5F6H
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

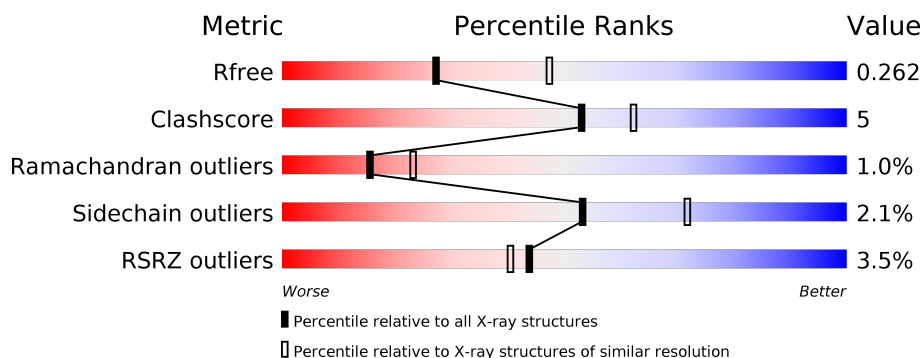
1 Overall quality at a glance

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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	<div> <div>12%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>••</div> </div> </div>
1	L	216	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>
1	N	216	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>
1	P	216	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div> </div>
2	I	227	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>7%</div> </div> </div>
2	K	227	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	M	227	<div><div></div><div>4%</div><div></div><div>79%</div><div></div><div>13%</div><div></div><div>7%</div></div>
2	O	227	<div><div></div><div>%</div><div></div><div>77%</div><div></div><div>15%</div><div></div><div>• 7%</div></div>

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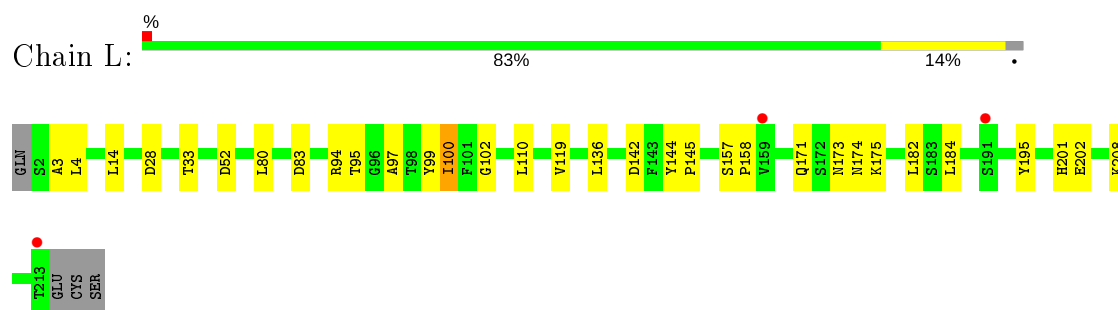
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	11	Total	O	0	0
			11	11		
3	M	23	Total	O	0	0
			23	23		
3	O	22	Total	O	0	0
			22	22		

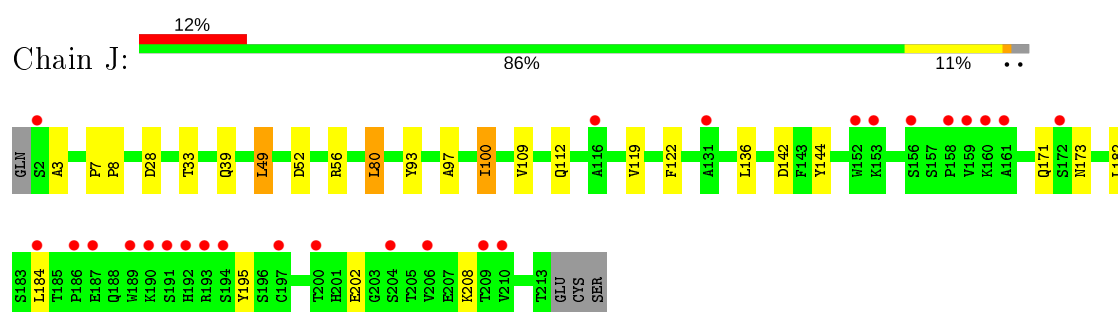
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

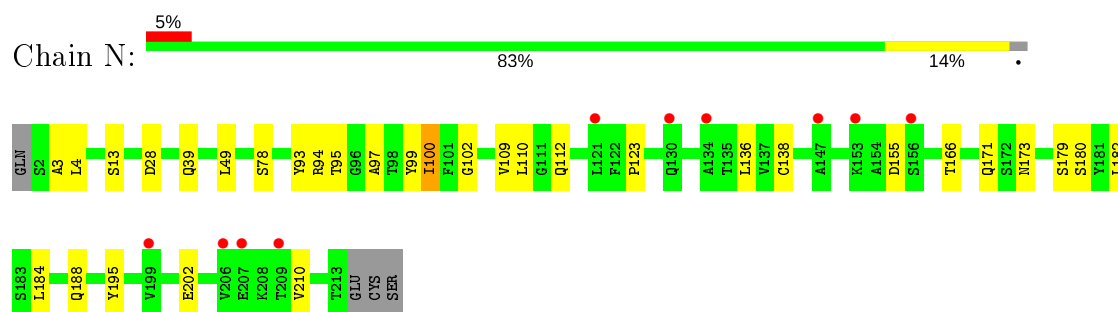
• Molecule 1: DH427 Antibody Light Chain



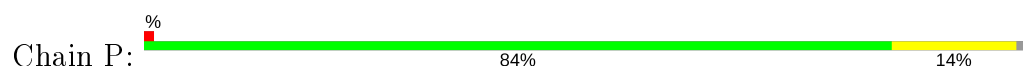
• Molecule 1: DH427 Antibody Light Chain

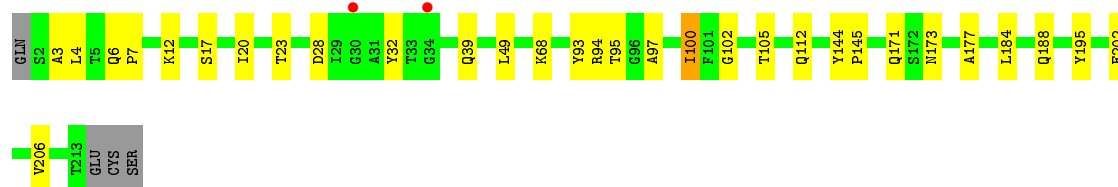


• Molecule 1: DH427 Antibody Light Chain

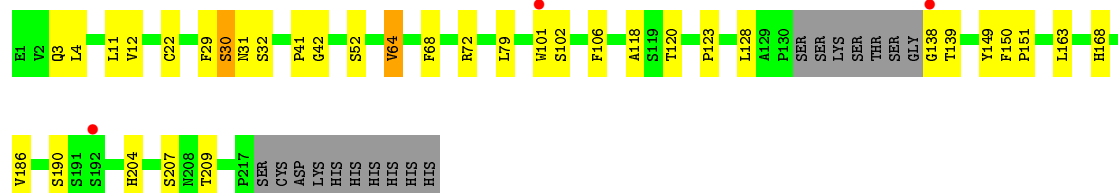
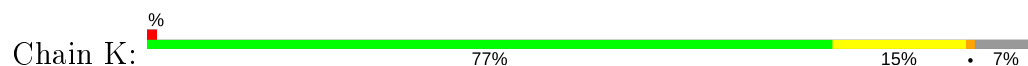


• Molecule 1: DH427 Antibody Light Chain

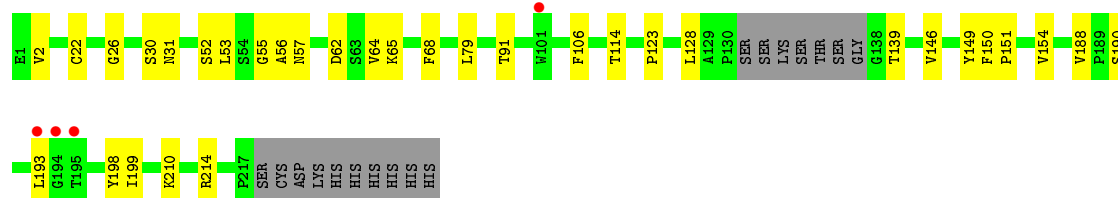
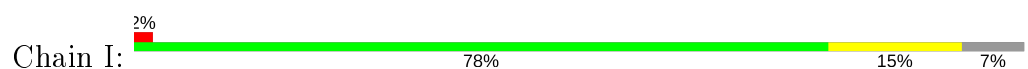




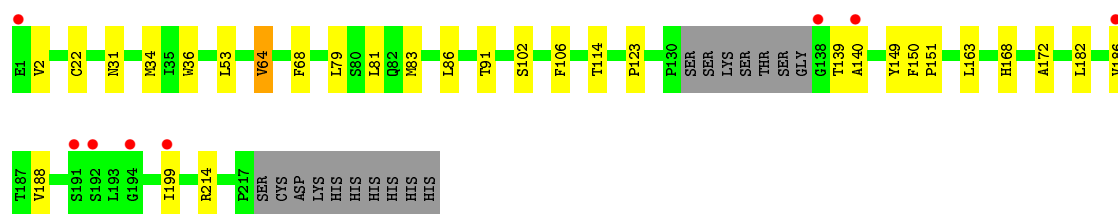
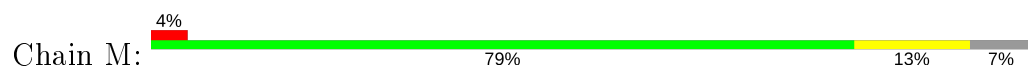
• Molecule 2: DH427 Antibody Heavy Chain



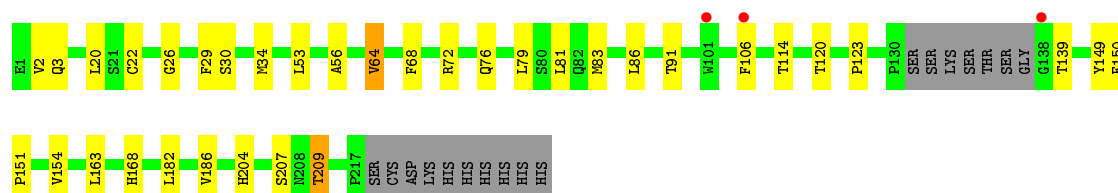
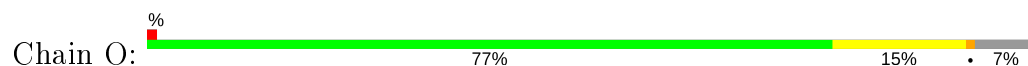
• Molecule 2: DH427 Antibody Heavy Chain



• 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 0.229 , 0.262	Depositor DCC
R_{free} test set	2861 reflections (5.16%)	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 , 20.3	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	0.26	0/1610	0.47	0/2198
1	L	0.28	0/1610	0.48	0/2198
1	N	0.25	0/1610	0.46	0/2198
1	P	0.27	0/1610	0.46	0/2198
2	I	0.27	0/1610	0.49	0/2193
2	K	0.28	0/1610	0.51	0/2193
2	M	0.27	0/1610	0.49	0/2193
2	O	0.27	0/1610	0.49	0/2193
All	All	0.27	0/12880	0.48	0/17564

There are no bond length outliers.

There are no bond angle outliers.

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	16	0
1	L	1574	0	1525	20	0
1	N	1574	0	1525	21	0
1	P	1574	0	1525	19	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	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	134	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 5.

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)
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
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: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
2:K:138:GLY:N	1:N:78:SER:HG	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:K:30:SER:C	2:K:32:SER:H	2.12	0.53
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
1:J:136:LEU:HD22	1:J:182:LEU:HD23	1.92	0.51
2:K:29:PHE:O	2:K:72:ARG:NH2	2.43	0.51
1:P:39:GLN:HB2	1:P:49:LEU:HD11	1.91	0.51
2:I:55:GLY:O	2:I:57:ASN:N	2.35	0.51
1:P:94:ARG:HG2	1:P:95:THR:H	1.75	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
2:I:62:ASP:O	2:I:65:LYS:HG2	2.13	0.49
1:N:109:VAL:O	1:N:112:GLN:NE2	2.40	0.49
2:I:31:ASN:HA	2:I:53:LEU:HD22	1.94	0.49
1:N:97:ALA:O	3:N:301:HOH:O	2.20	0.49
2:K:163:LEU:HD21	2:K:186:VAL:HG21	1.95	0.49
2:K:52:SER:O	2:K:72:ARG:NH1	2.45	0.49
2:I:91:THR:HG23	2:I:114:THR:HA	1.94	0.48
1:N:4:LEU:HB2	1:N:102:GLY:HA2	1.95	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:123:PRO:HB3	2:O:149:TYR:HB3	1.95	0.48
2:O:30:SER:O	2:O:53:LEU:HB2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:12:LYS:HD2	1:P:17:SER:O	2.14	0.47
1:J:33:THR:O	1:J:52:ASP:HA	2.15	0.47
1:L:171:GLN:HB2	1:L:173:ASN:OD1	2.15	0.47
2:K:204:HIS:HB3	2:K:209:THR:HB	1.96	0.46
1:L:184:LEU:HD21	1:L:195:TYR:CZ	2.50	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
2:M:123:PRO:HB3	2:M:149:TYR:HB3	1.96	0.46
1:P:112:GLN:HB2	1:P:144:TYR:CE2	2.50	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:N:171:GLN:HB2	1:N:173:ASN:OD1	2.16	0.45
1:N:39:GLN:HB2	1:N:49:LEU:HD11	1.96	0.45
1:L:14:LEU:HB3	1:P:206:VAL:HG12	1.97	0.45
2:O:22:CYS:HB3	2:O:79:LEU:HB3	1.98	0.45
2:O:2:VAL:HA	2:O:26:GLY:HA3	1.99	0.45
2:K:204:HIS:ND1	2:K:207:SER:OG	2.44	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
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:11:LEU:HD21	2:K:118:ALA:O	2.19	0.43
2:K:3:GLN:O	2:K:4:LEU:HD13	2.18	0.43
2:M:36:TRP:CE2	2:M:81:LEU:HB2	2.54	0.43
2:O:20:LEU:HD12	2:O:81:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:171:GLN:NE2	1:P:173:ASN:OD1	2.42	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
2:M:172:ALA:HA	2:M:182:LEU:HB3	2.00	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:O:120:THR:CG2	2:O:207:SER:HB3	2.50	0.41
1:P:32:TYR:O	1:P:68:LYS:NZ	2.54	0.41
2:K:41:PRO:HA	2:K:42:GLY:HA2	1.67	0.41
1:L:83:ASP:OD1	1:L:174:ASN:ND2	2.49	0.41
1:L:95:THR:C	1:L:97:ALA:H	2.24	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:J:7:PRO:HA	1:J:8:PRO:HD3	1.94	0.41
1:L:142:ASP:H	1:L:171:GLN:HE22	1.67	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
1:J:80:LEU:HA	1:J:80:LEU:HD12	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
2:O:91:THR:HG23	2:O:114:THR:HA	2.02	0.40
2:O:34:MET:HB3	2:O:79:LEU:HD22	2.02	0.40
1:P:6:GLN:HB3	1:P:105:THR:CG2	2.52	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%)	29	43
1	L	210/216 (97%)	201 (96%)	8 (4%)	1 (0%)	29	43
1	N	210/216 (97%)	196 (93%)	12 (6%)	2 (1%)	15	23
1	P	210/216 (97%)	200 (95%)	9 (4%)	1 (0%)	29	43
2	I	206/227 (91%)	196 (95%)	7 (3%)	3 (2%)	10	15
2	K	206/227 (91%)	193 (94%)	9 (4%)	4 (2%)	8	11
2	M	206/227 (91%)	196 (95%)	8 (4%)	2 (1%)	15	23
2	O	206/227 (91%)	194 (94%)	9 (4%)	3 (2%)	10	15
All	All	1664/1772 (94%)	1576 (95%)	71 (4%)	17 (1%)	15	23

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
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%)	43	61
1	L	179/183 (98%)	175 (98%)	4 (2%)	52	70
1	N	179/183 (98%)	177 (99%)	2 (1%)	73	85
1	P	179/183 (98%)	176 (98%)	3 (2%)	60	77
2	I	175/191 (92%)	173 (99%)	2 (1%)	73	85
2	K	175/191 (92%)	169 (97%)	6 (3%)	37	53
2	M	175/191 (92%)	172 (98%)	3 (2%)	60	77
2	O	175/191 (92%)	170 (97%)	5 (3%)	42	60
All	All	1416/1496 (95%)	1386 (98%)	30 (2%)	53	72

All (30) 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	12	VAL
2	K	64	VAL
2	K	101	TRP
2	K	128	LEU
2	K	168	HIS
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	30	SER
2	I	210	LYS
2	M	2	VAL
2	M	64	VAL
2	M	168	HIS

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Mol	Chain	Res	Type
2	O	3	GLN
2	O	64	VAL
2	O	76	GLN
2	O	168	HIS
2	O	209	THR

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

Mol	Chain	Res	Type
1	L	171	GLN
1	J	171	GLN
1	J	198	GLN
1	N	198	GLN
2	I	168	HIS
2	O	76	GLN
2	O	175	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 carbohydrates 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	J	212/216 (98%)	0.63	26 (12%) 4 2	10, 34, 70, 85	0
1	L	212/216 (98%)	0.25	3 (1%) 75 73	10, 24, 57, 77	0
1	N	212/216 (98%)	0.46	10 (4%) 31 28	9, 37, 64, 78	0
1	P	212/216 (98%)	0.11	2 (0%) 84 83	9, 28, 49, 61	0
2	I	210/227 (92%)	0.15	4 (1%) 66 63	9, 17, 52, 65	0
2	K	210/227 (92%)	0.07	3 (1%) 75 73	9, 16, 46, 64	0
2	M	210/227 (92%)	0.18	8 (3%) 40 36	10, 18, 55, 71	0
2	O	210/227 (92%)	0.17	3 (1%) 75 73	11, 20, 44, 73	0
All	All	1688/1772 (95%)	0.25	59 (3%) 44 40	9, 22, 59, 85	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	156	SER	4.2
1	J	193	ARG	4.2
1	N	207	GLU	4.2
1	J	194	SER	4.1
1	J	204	SER	4.0
2	O	138	GLY	3.7
1	J	186	PRO	3.5
1	J	159	VAL	3.2
2	O	101	TRP	3.1
1	J	2	SER	3.0
2	I	193	LEU	3.0
1	N	199	VAL	2.9
2	M	140	ALA	2.9
2	M	1	GLU	2.9
2	K	138	GLY	2.9
1	J	192	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	K	101	TRP	2.8
1	J	161	ALA	2.8
1	J	191	SER	2.7
1	J	187	GLU	2.7
2	M	191	SER	2.7
1	L	191	SER	2.7
1	J	197	CYS	2.7
2	I	195	THR	2.6
1	N	206	VAL	2.6
1	J	184	LEU	2.6
2	M	138	GLY	2.6
2	M	192	SER	2.6
1	L	213	THR	2.5
1	P	34	GLY	2.5
1	J	153	LYS	2.5
1	J	210	VAL	2.5
1	J	158	PRO	2.5
1	J	189	TRP	2.4
1	L	159	VAL	2.4
2	M	194	GLY	2.4
1	J	209	THR	2.4
1	J	116	ALA	2.3
2	O	106	PHE	2.3
1	N	147	ALA	2.3
1	J	190	LYS	2.3
2	I	194	GLY	2.2
2	K	192	SER	2.2
1	N	209	THR	2.2
2	M	186	VAL	2.2
1	N	130	GLN	2.2
1	J	172	SER	2.2
1	N	134	ALA	2.2
1	J	131	ALA	2.2
1	J	206	VAL	2.1
1	P	30	GLY	2.1
2	M	199	ILE	2.1
1	N	121	LEU	2.1
1	N	156	SER	2.1
1	J	160	LYS	2.0
1	J	152	TRP	2.0
1	N	153	LYS	2.0
2	I	101	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	200	THR	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 carbohydrates 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.