



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2021 – 08:02 am BST

PDB ID : 6XUL  
Title : Apo Ab 5b1  
Authors : Diskin, R.; Borenstein-Katz, A.  
Deposited on : 2020-01-20  
Resolution : 2.41 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

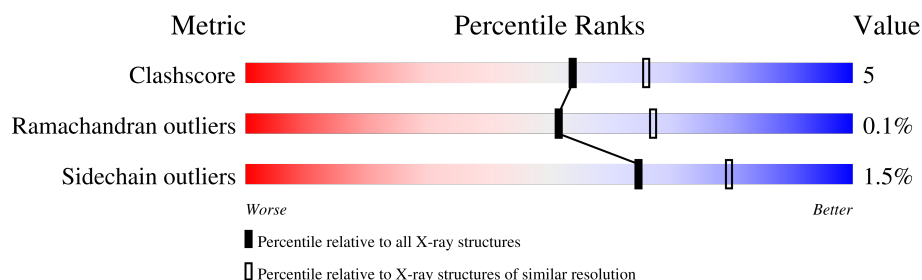
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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))
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)





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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	230	
1	C	230	
1	E	230	
1	G	230	
1	H	230	
1	J	230	
2	B	218	
2	D	218	

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Mol	Chain	Length	Quality of chain
2	F	218	 88%11%
2	I	218	 87%13%
2	K	218	 83%16%
2	L	218	 84%14%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20926 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 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	1	0
			1665	1051	288	319	7			
1	C	218	Total	C	N	O	S	0	1	0
			1665	1051	288	319	7			
1	E	218	Total	C	N	O	S	0	1	0
			1665	1051	288	319	7			
1	G	219	Total	C	N	O	S	0	0	0
			1668	1052	289	321	6			
1	J	218	Total	C	N	O	S	0	1	0
			1665	1051	288	319	7			
1	H	218	Total	C	N	O	S	0	1	0
			1665	1051	288	319	7			

- Molecule 2 is a protein called Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	1	0
			1651	1026	284	336	5			
2	D	217	Total	C	N	O	S	0	1	0
			1651	1026	284	336	5			
2	F	217	Total	C	N	O	S	0	1	0
			1651	1026	284	336	5			
2	I	217	Total	C	N	O	S	0	2	0
			1659	1031	287	336	5			
2	K	217	Total	C	N	O	S	0	0	0
			1648	1024	284	336	4			
2	L	217	Total	C	N	O	S	0	1	0
			1651	1026	284	336	5			

- Molecule 3 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total 138	O 138	0	0
3	B	130	Total 130	O 130	0	0
3	C	103	Total 103	O 103	0	0
3	D	54	Total 54	O 54	0	0
3	E	98	Total 98	O 98	0	0
3	F	62	Total 62	O 62	0	0
3	G	125	Total 125	O 125	0	0
3	I	89	Total 89	O 89	0	0
3	J	85	Total 85	O 85	0	0
3	K	35	Total 35	O 35	0	0
3	H	62	Total 62	O 62	0	0
3	L	41	Total 41	O 41	0	0

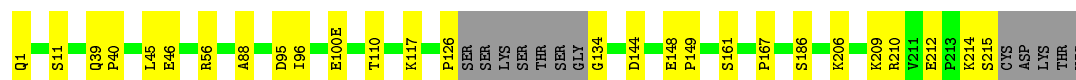
### 3 Residue-property plots [i](#)

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. 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. 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.


Note EDS was not executed.

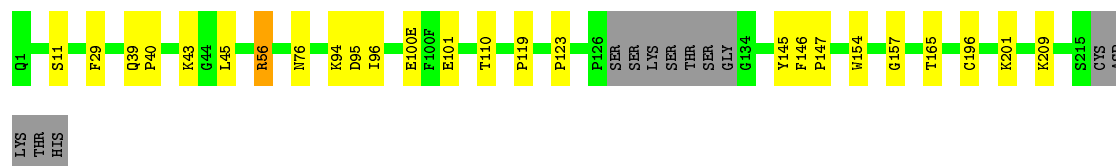
- Molecule 1: Heavy chain

Chain A: 




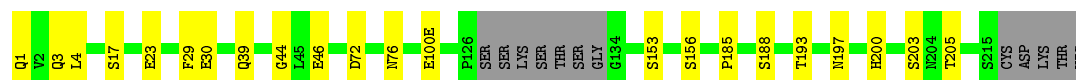
- Molecule 1: Heavy chain

Chain C: 




- Molecule 1: Heavy chain

Chain E: 




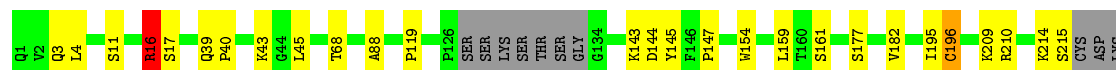
- Molecule 1: Heavy chain

Chain G: 




- Molecule 1: Heavy chain

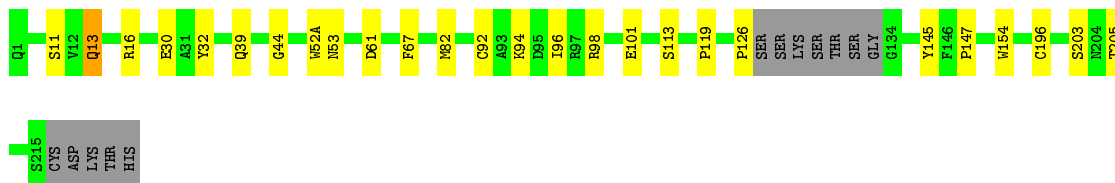
Chain J: 




THR  
HIS

• Molecule 1: Heavy chain

Chain H:  83% 11% 5%




• Molecule 2: Light chain

Chain B:  89% 11%



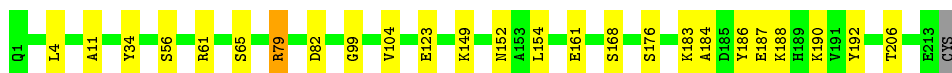
• Molecule 2: Light chain

Chain D:  87% 12%




• Molecule 2: Light chain

Chain F:  88% 11%




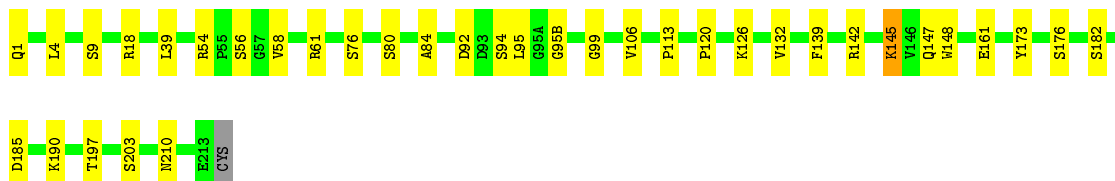
• Molecule 2: Light chain

Chain I:  87% 13%

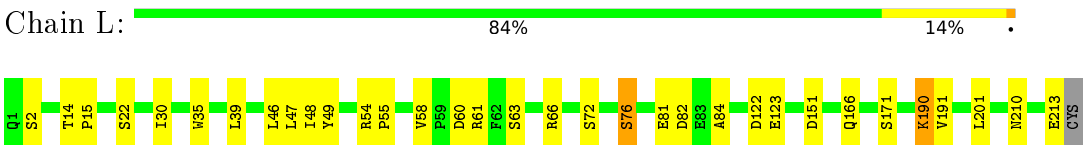


• Molecule 2: Light chain

Chain K:  83% 16%



● Molecule 2: Light chain





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.02Å 155.02Å 121.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.88 – 2.41	Depositor
% Data completeness (in resolution range)	99.7 (47.88-2.41)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.168 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

## 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	A	0.48	0/1709	0.63	0/2323
1	C	0.42	0/1709	0.60	0/2323
1	E	0.45	0/1709	0.61	0/2323
1	G	0.45	0/1709	0.61	0/2323
1	H	0.41	0/1709	0.59	0/2323
1	J	0.44	0/1709	0.59	1/2323 (0.0%)
2	B	0.42	0/1691	0.60	0/2300
2	D	0.38	0/1691	0.57	0/2300
2	F	0.41	0/1691	0.59	0/2300
2	I	0.42	0/1702	0.59	0/2314
2	K	0.38	0/1685	0.53	0/2292
2	L	0.38	0/1691	0.57	0/2300
All	All	0.42	0/20405	0.59	1/27744 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	16	ARG	NE-CZ-NH2	-5.03	117.79	120.30

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	A	1665	0	1624	21	0
1	C	1665	0	1624	19	0
1	E	1665	0	1624	16	0
1	G	1668	0	1625	17	0
1	H	1665	0	1624	19	0
1	J	1665	0	1624	17	0
2	B	1651	0	1588	17	0
2	D	1651	0	1588	17	0
2	F	1651	0	1588	16	0
2	I	1659	0	1601	15	0
2	K	1648	0	1584	20	0
2	L	1651	0	1588	19	0
3	A	138	0	0	7	0
3	B	130	0	0	6	0
3	C	103	0	0	5	0
3	D	54	0	0	4	0
3	E	98	0	0	7	1
3	F	62	0	0	4	0
3	G	125	0	0	9	1
3	H	62	0	0	3	0
3	I	89	0	0	2	0
3	J	85	0	0	4	0
3	K	35	0	0	6	0
3	L	41	0	0	6	0
All	All	20926	0	19282	207	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 (207) 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:E:193:THR:OG1	3:E:301:HOH:O	1.85	0.92
2:F:168:SER:OG	3:F:301:HOH:O	1.88	0.91
2:L:201:LEU:O	3:L:301:HOH:O	1.88	0.90
1:C:43:LYS:O	3:C:301:HOH:O	1.93	0.86
2:B:144:ALA:O	3:B:301:HOH:O	1.95	0.85
1:G:125:ALA:O	3:G:301:HOH:O	1.95	0.85
2:I:152:ASN:OD1	3:I:301:HOH:O	1.94	0.84
2:B:17:GLN:OE1	3:B:302:HOH:O	1.97	0.81
2:L:54:ARG:NH1	2:L:58:VAL:O	2.12	0.80
1:J:17:SER:O	3:J:301:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:190:LYS:HE2	2:I:210:ASN:HB3	1.67	0.77
2:B:93:ASP:OD2	3:B:304:HOH:O	2.04	0.76
1:E:72:ASP:OD2	3:E:302:HOH:O	2.06	0.73
1:C:96:ILE:O	3:C:302:HOH:O	2.06	0.73
1:E:203:SER:HG	1:E:205:THR:HG1	1.33	0.72
1:J:11:SER:HB2	1:J:147:PRO:HG3	1.71	0.72
1:C:157:GLY:O	3:C:303:HOH:O	2.06	0.72
1:J:4:LEU:O	3:J:302:HOH:O	2.08	0.71
1:E:46:GLU:OE1	3:E:303:HOH:O	2.08	0.71
1:E:4:LEU:O	3:E:304:HOH:O	2.09	0.70
2:F:123:GLU:OE1	3:F:302:HOH:O	2.09	0.70
2:K:56:SER:O	3:K:302:HOH:O	2.10	0.69
1:A:46:GLU:OE1	3:A:301:HOH:O	2.11	0.69
1:E:153:SER:HB2	1:E:197:ASN:HB2	1.73	0.69
1:C:94:LYS:NZ	1:C:101:GLU:OE1	2.22	0.68
2:K:120:PRO:HD3	2:K:132:VAL:HG22	1.76	0.68
2:K:9:SER:O	3:K:303:HOH:O	2.11	0.68
1:A:214:LYS:HG2	1:A:215:SER:H	1.59	0.67
2:D:39:LEU:HD23	2:D:84:ALA:HB2	1.74	0.67
1:C:96:ILE:HG12	1:C:101:GLU:HB2	1.76	0.66
1:A:134:GLY:N	3:A:305:HOH:O	2.29	0.66
1:G:115:SER:O	3:G:302:HOH:O	2.12	0.66
1:A:167:PRO:O	3:A:302:HOH:O	2.14	0.66
2:L:122:ASP:OD2	3:L:302:HOH:O	2.14	0.66
1:E:23:GLU:OE1	3:E:306:HOH:O	2.12	0.66
1:J:144:ASP:OD1	3:J:303:HOH:O	2.14	0.66
1:E:156:SER:OG	3:E:307:HOH:O	2.15	0.65
1:H:53:ASN:ND2	3:H:301:HOH:O	2.05	0.65
1:C:123:PRO:HD3	1:C:209:LYS:HE2	1.78	0.64
1:C:209:LYS:NZ	2:D:123:GLU:OE2	2.30	0.64
2:B:93:ASP:OD1	3:B:305:HOH:O	2.15	0.64
2:K:80:SER:HA	2:K:106:VAL:HG21	1.79	0.64
2:F:206:THR:OG1	3:F:303:HOH:O	2.15	0.63
1:A:117:LYS:NZ	3:A:309:HOH:O	2.32	0.62
1:H:13:GLN:HB2	1:H:16:ARG:HD2	1.81	0.62
2:L:30:ILE:O	2:L:66:ARG:NH1	2.33	0.61
1:A:144:ASP:OD1	3:A:303:HOH:O	2.16	0.60
2:D:188:LYS:HB2	2:D:188:LYS:HZ3	1.67	0.60
1:A:1:GLN:N	3:A:311:HOH:O	2.35	0.59
1:H:13:GLN:HG3	1:H:16:ARG:HH11	1.68	0.59
1:J:68:THR:OG1	3:J:304:HOH:O	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ASN:OD1	2:B:138:ASN:ND2	2.37	0.58
2:B:45:LYS:NZ	3:B:309:HOH:O	2.36	0.57
1:G:11:SER:HB2	1:G:147:PRO:HG3	1.86	0.57
1:A:1:GLN:N	1:A:1:GLN:OE1	2.34	0.57
1:A:100(E):GLU:OE1	2:B:34:TYR:OH	2.23	0.56
1:J:214:LYS:HG2	1:J:215:SER:N	2.20	0.56
2:D:29:ASN:OD1	2:D:30:ILE:N	2.32	0.56
1:H:96:ILE:HG12	1:H:101:GLU:HB2	1.87	0.55
1:A:214:LYS:HG2	1:A:215:SER:N	2.22	0.55
2:I:168:SER:OG	2:I:169:LYS:HE2	2.06	0.55
2:D:4:LEU:HB2	2:D:99:GLY:HA2	1.89	0.54
1:H:154:TRP:CH2	1:H:196:CYS:HB3	2.43	0.54
2:I:190:LYS:HE3	2:I:211:ARG:O	2.07	0.54
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.89	0.53
1:C:11:SER:HB3	1:C:147:PRO:HG3	1.90	0.53
1:G:1:GLN:NE2	3:G:308:HOH:O	2.35	0.53
2:D:210:ASN:ND2	3:D:302:HOH:O	2.24	0.52
1:A:96:ILE:HG22	1:A:100(E):GLU:HB2	1.90	0.52
2:I:21:ILE:HD12	2:I:73:LEU:HD23	1.92	0.52
2:K:1:GLN:NE2	3:K:310:HOH:O	2.42	0.52
1:J:40:PRO:HG2	1:J:43:LYS:HB2	1.91	0.52
1:A:210:ARG:HD2	1:A:212:GLU:OE1	2.10	0.51
2:L:122:ASP:N	3:L:306:HOH:O	2.41	0.51
1:A:126:PRO:O	3:A:304:HOH:O	2.19	0.51
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.93	0.51
1:E:185:PRO:O	1:E:188:SER:OG	2.28	0.51
1:G:105:GLN:NE2	3:G:305:HOH:O	2.23	0.51
1:H:30:GLU:O	1:H:52(A):TRP:HB2	2.11	0.51
1:H:126:PRO:O	3:H:302:HOH:O	2.18	0.51
2:D:9:SER:HB2	3:D:321:HOH:O	2.10	0.51
2:I:11:ALA:O	2:I:104:VAL:HA	2.11	0.51
2:K:4:LEU:HB2	2:K:99:GLY:HA2	1.93	0.51
2:L:46:LEU:HD11	2:L:49:TYR:HB3	1.92	0.50
1:G:127:SER:OG	3:G:304:HOH:O	2.19	0.50
2:F:161:GLU:HA	2:F:176:SER:O	2.12	0.50
2:F:4:LEU:HB2	2:F:99:GLY:HA2	1.93	0.50
1:J:39:GLN:HB2	1:J:45:LEU:HD23	1.93	0.50
1:E:100(E):GLU:OE1	2:F:34:TYR:OH	2.30	0.49
1:G:126:PRO:HA	1:G:137:ALA:O	2.13	0.49
2:D:184:ALA:O	2:D:188:LYS:HG3	2.13	0.49
1:C:56:ARG:HH11	1:C:56:ARG:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4:LEU:HB2	2:I:99:GLY:HA2	1.95	0.49
2:F:152:ASN:N	3:F:304:HOH:O	2.30	0.49
1:J:195:ILE:HD13	1:J:210:ARG:HA	1.94	0.49
2:L:151:ASP:OD1	2:L:190:LYS:HG3	2.13	0.48
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.94	0.48
1:E:1:GLN:OE1	1:E:1:GLN:N	2.45	0.48
1:J:159:LEU:HD21	1:J:182:VAL:HG21	1.95	0.48
1:H:13:GLN:HG3	1:H:16:ARG:NH1	2.28	0.48
1:H:39:GLN:HG3	1:H:44:GLY:O	2.14	0.48
2:F:65:SER:HB3	2:K:203:SER:HB3	1.96	0.48
2:L:61:ARG:HB3	2:L:76:SER:O	2.13	0.48
2:F:186:TYR:O	2:F:192:TYR:OH	2.32	0.48
1:G:100(E):GLU:OE1	2:I:34:TYR:OH	2.31	0.48
1:C:201:LYS:HG2	3:C:362:HOH:O	2.14	0.48
2:K:54:ARG:HD2	2:K:58:VAL:HG12	1.96	0.48
2:L:39:LEU:HD23	2:L:84:ALA:HB2	1.95	0.48
2:L:190:LYS:HD2	2:L:191:VAL:HG23	1.95	0.47
2:F:61:ARG:HH22	2:F:82:ASP:CG	2.18	0.47
1:J:119:PRO:HB3	1:J:145:TYR:HB3	1.96	0.47
2:K:113:PRO:HB3	2:K:139:PHE:HB3	1.95	0.47
1:H:94:LYS:NZ	1:H:101:GLU:OE1	2.39	0.47
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.97	0.46
1:G:39:GLN:HG3	1:G:44:GLY:O	2.14	0.46
2:K:61:ARG:HB3	2:K:76:SER:O	2.16	0.46
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.97	0.46
1:A:95:ASP:HA	1:A:100(E):GLU:O	2.16	0.46
1:G:123:PRO:HD3	1:G:209:LYS:HE2	1.97	0.46
2:I:166:GLN:HG2	2:I:171:SER:HA	1.98	0.46
1:E:30:GLU:CD	1:E:30:GLU:H	2.19	0.46
2:B:210:ASN:HB2	2:B:213:GLU:HG3	1.98	0.46
2:D:3:VAL:HG12	3:D:329:HOH:O	2.16	0.46
1:A:11:SER:HA	1:A:110:THR:O	2.16	0.46
1:A:148:GLU:OE1	1:A:149:PRO:HA	2.15	0.46
1:C:39:GLN:HB2	1:C:45:LEU:HD23	1.97	0.45
1:H:11:SER:HB2	1:H:147:PRO:HG3	1.97	0.45
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.99	0.45
2:D:11:ALA:O	2:D:104:VAL:HA	2.16	0.45
2:B:34:TYR:CE1	2:B:49:TYR:HB2	2.51	0.45
1:C:154:TRP:CH2	1:C:196:CYS:HB3	2.52	0.45
2:F:61:ARG:NH2	2:F:82:ASP:OD2	2.43	0.45
2:I:186:TYR:O	2:I:192:TYR:OH	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:SER:HA	2:B:106:VAL:HG21	1.97	0.45
1:C:165:THR:OG1	3:C:304:HOH:O	2.21	0.45
2:D:89:ALA:HB1	2:D:96:TYR:CE2	2.52	0.45
2:L:61:ARG:NH2	2:L:82:ASP:OD1	2.50	0.45
2:D:185:ASP:HA	2:D:188:LYS:HZ2	1.82	0.45
2:K:92:ASP:O	2:K:95(B):GLY:HA2	2.17	0.45
2:K:161:GLU:HA	2:K:176:SER:O	2.17	0.45
2:L:47:LEU:O	2:L:55:PRO:HD2	2.17	0.45
2:K:94:SER:OG	2:K:95:LEU:HG	2.17	0.44
2:D:163:VAL:HG22	2:D:175:LEU:HD12	1.99	0.44
1:H:30:GLU:OE1	1:H:30:GLU:N	2.46	0.44
2:B:54:ARG:NE	2:B:60:ASP:HA	2.32	0.44
1:C:11:SER:HA	1:C:110:THR:O	2.18	0.44
2:K:182:SER:N	3:K:307:HOH:O	2.28	0.44
2:L:123:GLU:HG3	3:L:306:HOH:O	2.18	0.44
2:K:39:LEU:HD23	2:K:84:ALA:HB2	1.98	0.44
1:G:64:LYS:HE2	1:G:64:LYS:HB2	1.75	0.44
2:K:148:TRP:N	3:K:301:HOH:O	1.87	0.44
1:H:96:ILE:O	3:H:303:HOH:O	2.21	0.44
2:L:210:ASN:ND2	3:L:311:HOH:O	2.51	0.44
1:J:40:PRO:HA	1:J:88:ALA:HA	1.99	0.44
1:E:29:PHE:CD2	1:E:76:ASN:HA	2.52	0.43
1:G:209:LYS:NZ	3:G:314:HOH:O	2.48	0.43
1:H:13:GLN:OE1	1:H:113:SER:HA	2.18	0.43
1:A:206:LYS:HE3	1:A:206:LYS:HB2	1.74	0.43
2:B:1:GLN:HG2	2:B:2:SER:N	2.33	0.43
1:J:143:LYS:HA	1:J:177:SER:OG	2.18	0.43
1:E:17:SER:O	3:E:308:HOH:O	2.20	0.43
1:E:39:GLN:HG3	1:E:44:GLY:O	2.18	0.43
2:I:190:LYS:HA	2:I:190:LYS:HD2	1.79	0.43
1:A:40:PRO:HA	1:A:88:ALA:HA	2.01	0.43
1:G:192:GLN:NE2	3:G:313:HOH:O	2.45	0.43
2:K:142:ARG:HD3	2:K:173:TYR:CE2	2.54	0.43
1:H:203:SER:OG	1:H:205:THR:OG1	2.34	0.42
1:G:214:LYS:HG2	1:G:215:SER:H	1.84	0.42
2:L:210:ASN:ND2	3:L:313:HOH:O	2.52	0.42
2:D:32:PHE:HB3	2:D:50:ARG:HA	2.00	0.42
1:H:32:TYR:CE1	1:H:98:ARG:HG3	2.55	0.42
2:K:145:LYS:HB2	2:K:197:THR:HB	2.02	0.42
2:D:18:ARG:NH2	3:D:307:HOH:O	2.38	0.42
2:D:61:ARG:HB2	2:D:76:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:81:GLU:OE1	2:L:81:GLU:N	2.31	0.42
2:L:166:GLN:HG2	2:L:171:SER:HA	2.01	0.42
2:K:190:LYS:HG2	2:K:210:ASN:HD22	1.84	0.42
1:C:40:PRO:HG2	1:C:43:LYS:HB2	2.02	0.41
1:J:16:ARG:HG2	1:J:16:ARG:HH11	1.84	0.41
2:K:147:GLN:HA	3:K:301:HOH:O	2.20	0.41
2:B:188:LYS:HG3	2:B:189:HIS:CE1	2.55	0.41
2:D:143:GLU:OE1	2:D:143:GLU:N	2.38	0.41
1:E:200:HIS:HB3	1:E:205:THR:HB	2.03	0.41
1:J:16:ARG:HH11	1:J:16:ARG:CG	2.32	0.41
2:L:14:THR:HG23	2:L:15:PRO:HD2	2.02	0.41
1:C:95:ASP:HA	1:C:100(E):GLU:O	2.21	0.41
2:F:183:LYS:HE3	2:F:187:GLU:OE1	2.20	0.41
1:G:192:GLN:HB2	3:G:313:HOH:O	2.20	0.41
1:H:154:TRP:CZ3	1:H:196:CYS:HB3	2.55	0.41
2:F:149:LYS:CG	2:F:154:LEU:HD23	2.51	0.41
1:G:213:PRO:HA	3:G:303:HOH:O	2.19	0.41
1:J:209:LYS:HD3	1:J:209:LYS:HA	1.78	0.41
2:F:61:ARG:HD3	2:F:79:ARG:NH1	2.35	0.41
2:I:59:PRO:HB2	2:I:61:ARG:HG2	2.03	0.41
2:I:145:LYS:HB3	2:I:197:THR:HB	2.02	0.41
2:I:163:VAL:HG22	2:I:175:LEU:HD12	2.02	0.41
1:H:67:PHE:CE1	1:H:82:MET:HB3	2.55	0.41
2:B:54:ARG:NE	3:B:303:HOH:O	2.01	0.41
1:A:134:GLY:C	1:A:186:SER:HG	2.25	0.40
1:A:209:LYS:NZ	2:B:123:GLU:OE2	2.54	0.40
1:C:146:PHE:HA	1:C:147:PRO:HA	1.87	0.40
1:C:29:PHE:CD2	1:C:76:ASN:HA	2.56	0.40
1:G:36:TRP:HD1	1:G:69:ILE:HD12	1.87	0.40
2:I:142:ARG:NH1	3:I:312:HOH:O	2.54	0.40
1:J:154:TRP:CH2	1:J:196:CYS:HB3	2.56	0.40
2:F:184:ALA:O	2:F:188:LYS:HG3	2.21	0.40
2:F:11:ALA:O	2:F:104:VAL:HA	2.22	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:E:348:HOH:O	3:G:421:HOH:O[2_545]	2.08	0.12



## 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	215/230 (94%)	211 (98%)	4 (2%)	0	100	100
1	C	215/230 (94%)	207 (96%)	8 (4%)	0	100	100
1	E	215/230 (94%)	205 (95%)	10 (5%)	0	100	100
1	G	215/230 (94%)	209 (97%)	5 (2%)	1 (0%)	29	40
1	H	215/230 (94%)	209 (97%)	6 (3%)	0	100	100
1	J	215/230 (94%)	209 (97%)	6 (3%)	0	100	100
2	B	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
2	D	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
2	F	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
2	I	217/218 (100%)	209 (96%)	6 (3%)	2 (1%)	17	24
2	K	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	L	216/218 (99%)	205 (95%)	11 (5%)	0	100	100
All	All	2586/2688 (96%)	2497 (97%)	86 (3%)	3 (0%)	51	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	126	PRO
2	I	77	GLY
2	I	212	GLY

### 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	184/194 (95%)	182 (99%)	2 (1%)	73	86
1	C	184/194 (95%)	183 (100%)	1 (0%)	88	95
1	E	184/194 (95%)	183 (100%)	1 (0%)	88	95
1	G	184/194 (95%)	182 (99%)	2 (1%)	73	86
1	H	184/194 (95%)	181 (98%)	3 (2%)	62	78
1	J	184/194 (95%)	180 (98%)	4 (2%)	52	69
2	B	187/187 (100%)	186 (100%)	1 (0%)	88	95
2	D	187/187 (100%)	185 (99%)	2 (1%)	73	86
2	F	187/187 (100%)	184 (98%)	3 (2%)	62	78
2	I	188/187 (100%)	186 (99%)	2 (1%)	73	86
2	K	186/187 (100%)	182 (98%)	4 (2%)	52	69
2	L	187/187 (100%)	179 (96%)	8 (4%)	29	44
All	All	2226/2286 (97%)	2193 (98%)	33 (2%)	65	79

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	161	SER
2	B	70	SER
1	C	56	ARG
2	D	67	SER
2	D	122	ASP
1	E	3	GLN
2	F	56	SER
2	F	79	ARG
2	F	190	LYS
1	G	56	ARG
1	G	197	ASN
2	I	2	SER
2	I	213	GLU
1	J	3	GLN
1	J	16	ARG
1	J	161	SER
1	J	196	CYS
2	K	18	ARG
2	K	126	LYS
2	K	145	LYS
2	K	185	ASP

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Mol	Chain	Res	Type
1	H	13	GLN
1	H	61	ASP
1	H	92	CYS
2	L	2	SER
2	L	22	SER
2	L	60	ASP
2	L	63	SER
2	L	72	SER
2	L	76	SER
2	L	190	LYS
2	L	213	GLU

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

Mol	Chain	Res	Type
2	B	17	GLN
2	D	189	HIS
1	G	164	HIS
2	I	137	ASN
2	K	210	ASN
2	L	95(C)	HIS

### 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 monosaccharides 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.