



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2026 – 02:17 PM EDT

PDB ID : 11HB / pdb\_000011hb  
Title : Crystal structure of a GII.4 norovirus capsid P domain in complex with neutralizing antibody 17A5  
Authors : Ghosh, A.; DuBois, R.M.  
Deposited on : 2026-02-23  
Resolution : 3.36 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

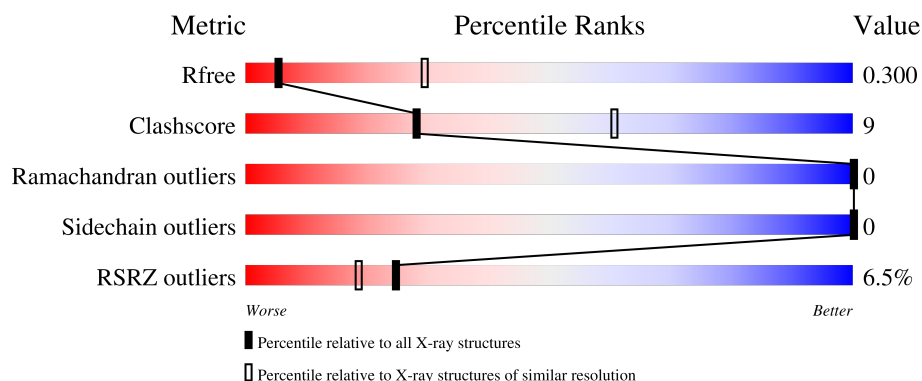
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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  $\leq 5\%$ . 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	311	<div> <div>2%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	B	311	<div> <div>3%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	E	311	<div> <div>2%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	C	225	<div> <div>8%</div> <div>70%</div> <div>25%</div> <div>5%</div> </div>
2	K	225	<div> <div>16%</div> <div>53%</div> <div>24%</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
2	L	225	<div><div></div><div>7%</div><div>74%</div><div>22%</div><div></div></div>
3	D	224	<div><div></div><div>7%</div><div>75%</div><div>16%</div><div>10%</div></div>
3	G	224	<div><div></div><div>9%</div><div>61%</div><div>20%</div><div>20%</div></div>
3	H	224	<div><div></div><div>4%</div><div>77%</div><div>16%</div><div>7%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16393 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 Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2405	1523	412	459	11			
1	B	307	Total	C	N	O	S	0	0	0
			2405	1523	412	459	11			
1	E	307	Total	C	N	O	S	0	0	0
			2405	1523	412	459	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLY	-	expression tag	UNP A0A1P8DD09
B	220	GLY	-	expression tag	UNP A0A1P8DD09
E	220	GLY	-	expression tag	UNP A0A1P8DD09

- Molecule 2 is a protein called 17A5 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1673	1050	282	334	7			
2	C	213	Total	C	N	O	S	0	0	0
			1653	1038	276	332	7			
2	K	173	Total	C	N	O	S	0	0	0
			1330	843	218	263	6			

- Molecule 3 is a protein called 17A5 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	208	Total	C	N	O	S	0	0	0
			1589	1009	257	317	6			
3	D	202	Total	C	N	O	S	0	0	0
			1544	983	249	307	5			

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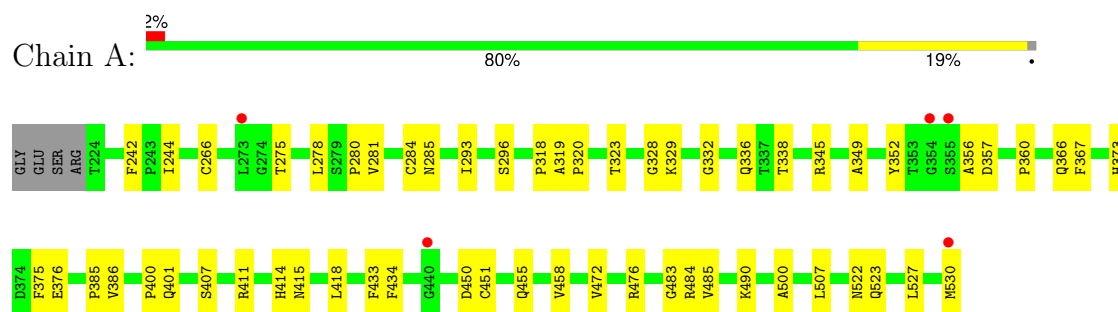
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	180	Total	C	N	O	S	0	0	0
			1389	885	225	274	5			

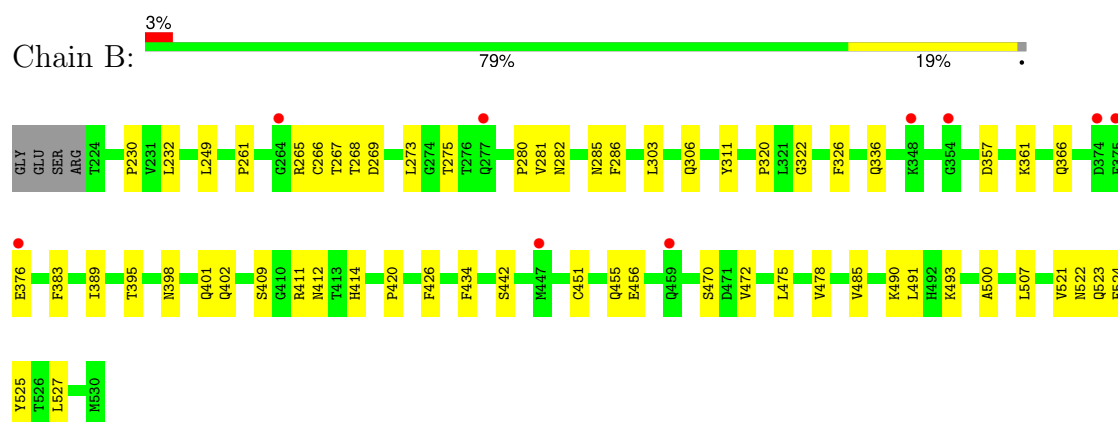
### 3 Residue-property plots [i](#)

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.

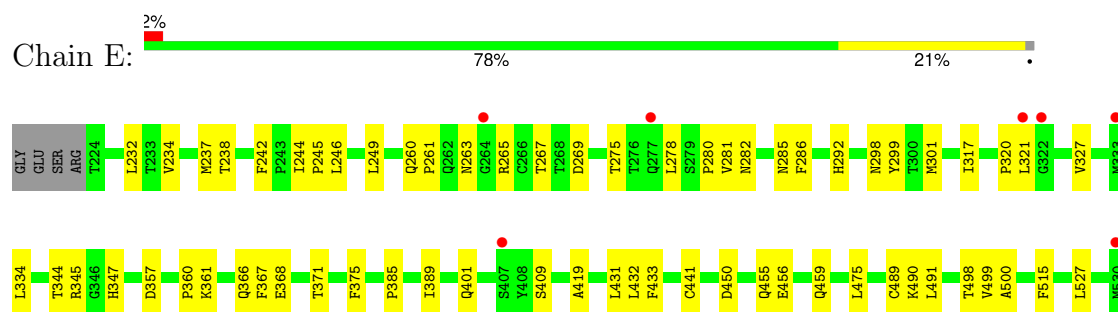
#### • Molecule 1: Major capsid protein VP1



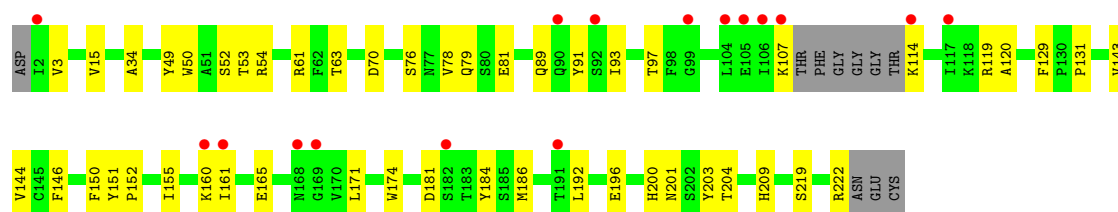
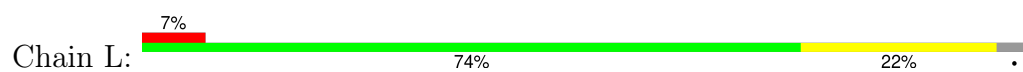
#### • Molecule 1: Major capsid protein VP1



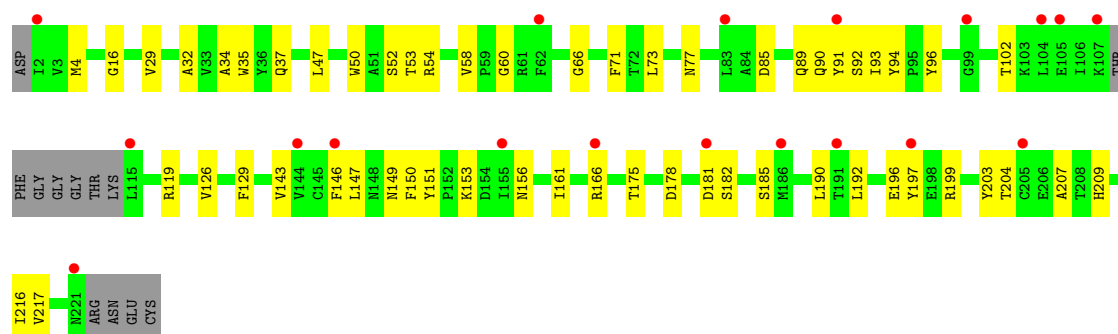
#### • Molecule 1: Major capsid protein VP1



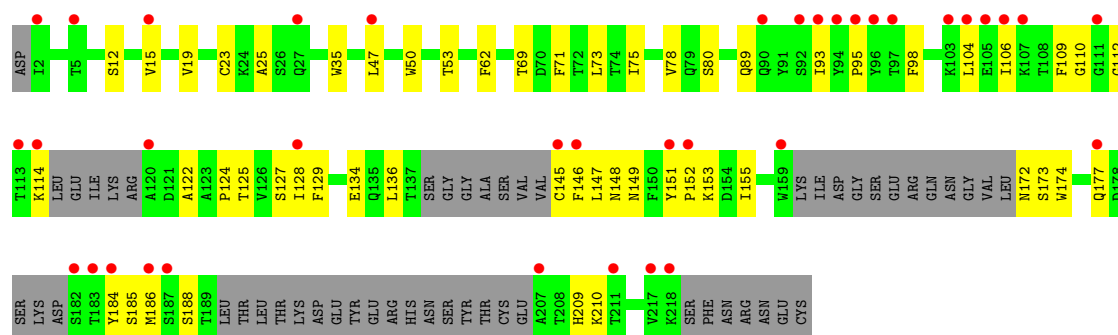
#### • Molecule 2: 17A5 Light Chain



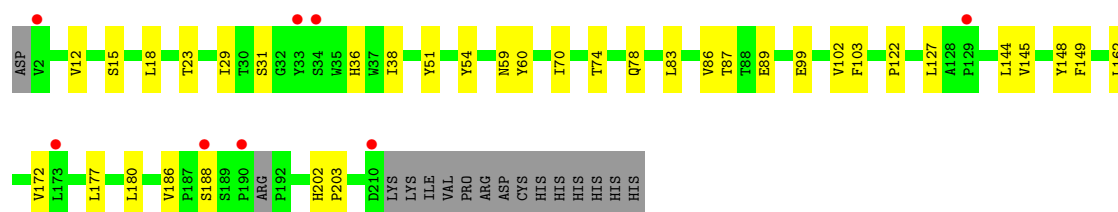
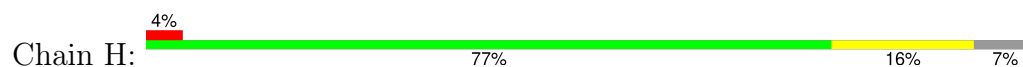
• Molecule 2: 17A5 Light Chain



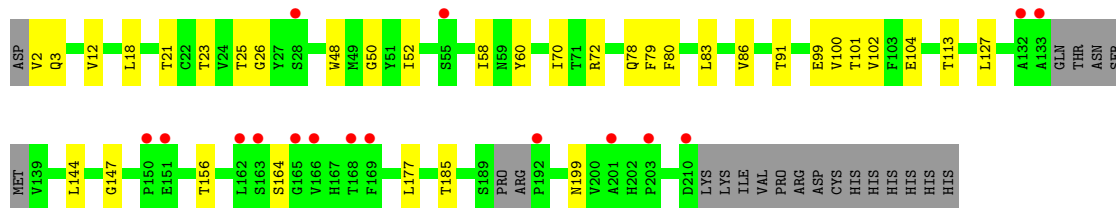
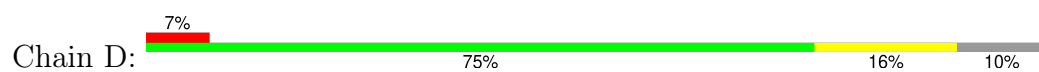
• Molecule 2: 17A5 Light Chain



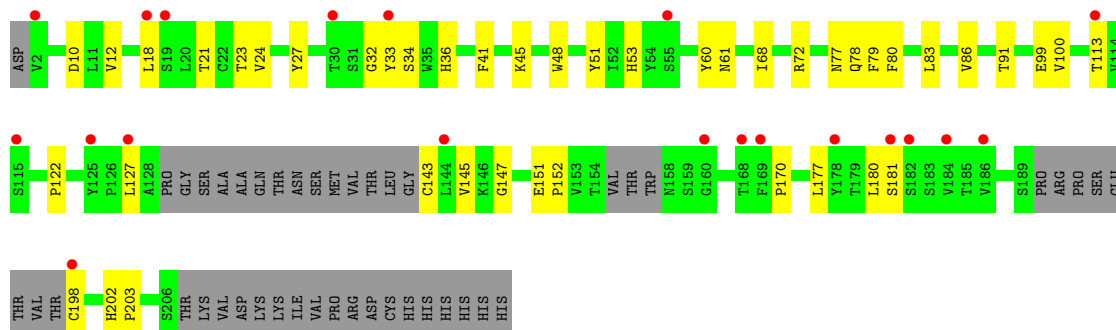
• Molecule 3: 17A5 Heavy Chain



• Molecule 3: 17A5 Heavy Chain



• Molecule 3: 17A5 Heavy Chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	271.95Å 134.91Å 133.91Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	48.43 – 3.36 48.43 – 3.36	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.43-3.36) 98.3 (48.43-3.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.258 , 0.300 0.258 , 0.300	Depositor DCC
$R_{free}$ test set	3439 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 80.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	16393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.11	0/2476	0.27	0/3387
1	B	0.09	0/2476	0.24	0/3387
1	E	0.09	0/2476	0.23	0/3387
2	C	0.11	0/1691	0.28	0/2294
2	K	0.12	0/1361	0.30	0/1844
2	L	0.10	0/1711	0.27	0/2319
3	D	0.11	0/1586	0.32	0/2172
3	G	0.14	0/1426	0.31	0/1948
3	H	0.13	0/1633	0.28	0/2238
All	All	0.11	0/16836	0.27	0/22976

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	A	2405	0	2296	37	0
1	B	2405	0	2296	39	0
1	E	2405	0	2296	43	0
2	C	1653	0	1588	42	0
2	K	1330	0	1272	39	0
2	L	1673	0	1614	32	0
3	D	1544	0	1497	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1389	0	1340	30	0
3	H	1589	0	1540	26	0
All	All	16393	0	15739	287	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 9.

All (287) 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:K:93:ILE:HG22	2:K:95:PRO:HD2	1.53	0.90
2:K:106:ILE:HD13	2:K:110:GLY:HA2	1.62	0.82
2:C:90:GLN:NE2	2:C:93:ILE:H	1.79	0.80
2:C:90:GLN:HE22	2:C:93:ILE:H	1.32	0.78
1:E:286:PHE:HB3	1:E:301:MET:HE1	1.66	0.76
2:K:173:SER:HB3	3:G:170:PRO:HG2	1.69	0.75
2:C:178:ASP:HB2	2:C:182:SER:H	1.54	0.72
2:L:160:LYS:HB2	2:L:204:THR:HB	1.70	0.72
1:E:261:PRO:HG2	1:E:265:ARG:HD3	1.71	0.71
2:K:155:ILE:HG21	2:K:186:MET:HE1	1.72	0.71
1:B:475:LEU:HD11	1:B:491:LEU:HD12	1.72	0.71
2:L:54:ARG:HH21	2:L:63:THR:HG22	1.56	0.71
1:A:357:ASP:HB3	1:A:366:GLN:HG3	1.74	0.68
3:G:91:THR:HG23	3:G:113:THR:HA	1.76	0.68
3:G:143:CYS:SG	3:G:198:CYS:N	2.67	0.67
1:E:281:VAL:O	1:E:285:ASN:ND2	2.27	0.67
2:C:149:ASN:ND2	2:C:181:ASP:OD2	2.28	0.66
2:L:161:ILE:HB	2:L:165:GLU:HB2	1.77	0.66
3:G:152:PRO:HB2	3:G:203:PRO:HG2	1.77	0.66
2:C:4:MET:HE2	2:C:90:GLN:HB2	1.77	0.66
1:A:280:PRO:HB3	1:A:455:GLN:HG2	1.78	0.66
2:C:161:ILE:HG21	2:C:166:ARG:HH21	1.60	0.66
1:A:411:ARG:NH1	3:H:99:GLU:OE2	2.30	0.64
2:L:49:TYR:HB2	3:H:102:VAL:HG21	1.80	0.64
3:G:23:THR:HA	3:G:78:GLN:HG2	1.78	0.64
1:A:275:THR:HG23	1:A:318:PRO:HG2	1.79	0.64
1:E:280:PRO:HB3	1:E:455:GLN:HG2	1.80	0.64
2:C:119:ARG:HH22	2:C:151:TYR:HA	1.62	0.64
1:E:389:ILE:HG22	1:E:441:CYS:HB2	1.78	0.64
3:G:12:VAL:HG11	3:G:18:LEU:HD11	1.80	0.63
3:H:15:SER:O	2:K:80:SER:OG	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:PRO:HG2	1:B:265:ARG:HD3	1.80	0.63
1:A:329:LYS:HG2	1:A:352:TYR:HD1	1.64	0.62
2:L:131:PRO:HD3	2:L:143:VAL:HG22	1.81	0.62
1:B:521:VAL:HG11	1:B:525:TYR:HB2	1.82	0.61
2:C:166:ARG:HH12	2:C:192:LEU:HD22	1.66	0.61
1:B:273:LEU:HD21	1:B:420:PRO:HD2	1.82	0.61
1:E:238:THR:HA	1:E:245:PRO:HA	1.82	0.61
1:E:433:PHE:HB3	1:E:450:ASP:HB3	1.83	0.60
2:K:172:ASN:HA	2:K:188:SER:HA	1.82	0.60
2:C:34:ALA:HB3	2:C:89:GLN:HG2	1.83	0.60
1:E:490:LYS:HG3	1:E:527:LEU:HD11	1.84	0.60
2:C:54:ARG:HH12	2:C:60:GLY:HA2	1.68	0.59
2:K:174:TRP:HD1	2:K:186:MET:HB2	1.67	0.59
2:C:119:ARG:NH2	2:C:151:TYR:HA	2.17	0.59
3:G:147:GLY:HA2	3:G:177:LEU:HB3	1.84	0.59
3:G:48:TRP:HE3	3:G:61:ASN:HD22	1.51	0.59
1:A:472:VAL:HG11	1:A:490:LYS:HD2	1.85	0.58
3:D:18:LEU:HD13	3:D:86:VAL:HG11	1.85	0.58
3:D:52:ILE:HD12	3:D:70:ILE:HG22	1.84	0.58
3:H:87:THR:HB	3:H:89:GLU:HG2	1.86	0.58
2:K:109:PHE:HE2	2:K:112:GLY:HA3	1.69	0.58
3:G:18:LEU:HD13	3:G:86:VAL:HG11	1.85	0.58
3:G:12:VAL:HG11	3:G:18:LEU:HD21	1.86	0.57
1:B:478:VAL:HA	1:B:485:VAL:HA	1.86	0.57
1:E:292:HIS:HA	1:E:299:TYR:HD1	1.68	0.57
3:D:52:ILE:HG13	3:D:58:ILE:HG12	1.87	0.57
1:A:490:LYS:HG3	1:A:527:LEU:HD11	1.85	0.57
2:C:90:GLN:HE21	2:C:92:SER:N	2.03	0.57
1:B:411:ARG:NH1	3:D:99:GLU:OE2	2.38	0.57
3:G:60:TYR:HB3	3:G:68:ILE:HD11	1.87	0.56
1:A:401:GLN:NE2	2:L:53:THR:OG1	2.33	0.56
2:L:3:VAL:HA	2:L:97:THR:HG21	1.88	0.56
1:B:401:GLN:OE1	2:C:53:THR:OG1	2.24	0.56
2:C:153:LYS:O	2:C:156:ASN:ND2	2.38	0.56
1:A:332:GLY:HA2	1:A:386:VAL:HG12	1.88	0.55
1:A:500:ALA:HB2	1:A:527:LEU:HB2	1.89	0.55
3:H:23:THR:HA	3:H:78:GLN:HG2	1.87	0.55
1:E:278:LEU:O	1:E:459:GLN:NE2	2.36	0.55
3:G:27:TYR:HE2	3:G:32:GLY:HA2	1.71	0.55
1:A:476:ARG:HD3	1:A:485:VAL:HG11	1.89	0.55
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ASN:ND2	1:B:306:GLN:OE1	2.40	0.55
3:G:34:SER:HB3	3:G:99:GLU:HB3	1.88	0.54
3:D:72:ARG:HA	3:D:79:PHE:HA	1.87	0.54
2:L:144:VAL:HG21	3:H:127:LEU:HD13	1.89	0.54
1:B:357:ASP:HB3	1:B:366:GLN:HG3	1.89	0.54
2:K:134:GLU:HG2	2:K:136:LEU:H	1.71	0.54
1:A:414:HIS:HB2	2:L:93:ILE:HD11	1.89	0.54
2:K:125:THR:O	2:K:147:LEU:HA	2.08	0.54
1:E:500:ALA:HB2	1:E:527:LEU:HB2	1.90	0.53
1:B:326:PHE:HB2	1:B:402:GLN:HA	1.90	0.53
1:E:357:ASP:HB3	1:E:366:GLN:HG3	1.91	0.53
1:B:280:PRO:HB3	1:B:455:GLN:HG2	1.91	0.53
1:A:407:SER:HB3	1:A:411:ARG:H	1.73	0.52
2:C:54:ARG:NH1	2:C:60:GLY:HA2	2.24	0.52
3:H:145:VAL:HB	3:H:180:LEU:HG	1.90	0.52
1:E:298:ASN:HB3	1:E:368:GLU:HA	1.91	0.52
1:B:336:GLN:HE22	1:B:376:GLU:H	1.57	0.52
2:C:143:VAL:HG22	2:C:190:LEU:HD11	1.90	0.52
3:D:127:LEU:HD11	3:D:144:LEU:HB2	1.91	0.52
1:A:522:ASN:O	1:A:523:GLN:HG2	2.10	0.52
1:E:232:LEU:HD22	1:E:456:GLU:HG2	1.91	0.52
2:C:47:LEU:HA	2:C:58:VAL:HG21	1.92	0.52
3:G:83:LEU:HD22	3:G:86:VAL:HG12	1.92	0.52
1:A:296:SER:HA	3:H:31:SER:HB3	1.91	0.51
2:K:151:TYR:HD2	2:K:153:LYS:HG3	1.74	0.51
3:G:41:PHE:HB2	3:G:45:LYS:HB2	1.91	0.51
2:L:204:THR:HG23	2:L:219:SER:HB2	1.93	0.51
3:D:12:VAL:HG11	3:D:18:LEU:HD11	1.92	0.51
1:B:490:LYS:HG3	1:B:527:LEU:HD11	1.91	0.51
1:B:472:VAL:HG11	1:B:490:LYS:HD2	1.93	0.51
1:B:389:ILE:HG13	1:B:442:SER:HB2	1.92	0.51
1:B:500:ALA:HB2	1:B:527:LEU:HB2	1.93	0.51
2:L:70:ASP:OD1	2:L:70:ASP:N	2.43	0.51
1:E:401:GLN:NE2	2:K:53:THR:OG1	2.35	0.50
1:E:263:ASN:ND2	1:E:275:THR:O	2.40	0.50
2:C:85:ASP:HA	2:C:102:THR:HA	1.92	0.50
3:G:33:TYR:CD1	3:G:100:VAL:HG12	2.46	0.50
2:L:150:PHE:O	2:L:184:TYR:N	2.45	0.50
2:K:153:LYS:HD3	2:K:210:LYS:HB3	1.94	0.50
1:B:282:ASN:HA	1:B:285:ASN:HD22	1.75	0.50
2:K:153:LYS:HD2	2:K:209:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:192:LEU:HD23	2:L:196:GLU:HB3	1.94	0.50
1:B:267:THR:OG1	1:B:269:ASP:OD1	2.20	0.50
3:D:60:TYR:HE1	3:D:70:ILE:HG13	1.77	0.49
3:D:2:VAL:HA	3:D:26:GLY:HA3	1.94	0.49
2:K:25:ALA:HB3	2:K:69:THR:HA	1.93	0.49
2:K:19:VAL:HG22	2:K:75:ILE:HB	1.95	0.49
1:E:489:CYS:HB3	1:E:499:VAL:HG12	1.93	0.49
2:K:148:ASN:O	2:K:185:SER:OG	2.27	0.49
3:H:102:VAL:HG12	3:H:103:PHE:H	1.78	0.49
2:C:197:TYR:O	2:C:203:TYR:OH	2.31	0.49
2:L:34:ALA:HB3	2:L:89:GLN:HG2	1.95	0.48
1:E:334:LEU:HB3	1:E:375:PHE:HZ	1.78	0.48
3:G:180:LEU:HD23	3:G:181:SER:N	2.28	0.48
1:B:412:ASN:HB3	2:C:94:TYR:HD2	1.78	0.48
1:B:266:CYS:SG	1:B:267:THR:N	2.86	0.48
1:B:281:VAL:O	1:B:285:ASN:ND2	2.46	0.48
1:E:357:ASP:OD2	3:G:53:HIS:NE2	2.46	0.48
1:B:268:THR:HG23	1:B:493:LYS:HA	1.94	0.48
2:K:151:TYR:CG	2:K:152:PRO:HD2	2.49	0.48
3:H:38:ILE:HD11	3:H:103:PHE:CE2	2.48	0.48
1:E:317:ILE:O	1:E:361:LYS:NZ	2.40	0.48
1:E:344:THR:O	1:E:345:ARG:NH1	2.42	0.48
3:G:21:THR:HA	3:G:80:PHE:CD1	2.49	0.48
1:A:349:ALA:HB1	1:A:367:PHE:HB3	1.96	0.48
1:A:483:GLY:O	1:B:523:GLN:NE2	2.47	0.48
2:L:201:ASN:HA	2:L:222:ARG:HB3	1.95	0.48
2:L:129:PHE:HE2	2:L:146:PHE:HD2	1.61	0.47
1:B:282:ASN:HA	1:B:285:ASN:ND2	2.29	0.47
1:E:267:THR:OG1	1:E:269:ASP:OD1	2.27	0.47
3:G:72:ARG:HA	3:G:79:PHE:HA	1.96	0.47
1:B:286:PHE:HB2	1:B:383:PHE:HB3	1.96	0.47
3:D:101:THR:HG23	3:D:102:VAL:HG13	1.95	0.47
3:G:24:VAL:O	3:G:77:ASN:ND2	2.47	0.47
1:A:373:HIS:O	1:A:375:PHE:N	2.42	0.47
2:L:61:ARG:HB3	2:L:76:SER:O	2.14	0.47
1:E:260:GLN:NE2	1:E:419:ALA:O	2.40	0.47
1:E:292:HIS:HA	1:E:299:TYR:CD1	2.47	0.47
2:K:146:PHE:HE2	3:G:127:LEU:HD11	1.78	0.47
3:G:10:ASP:OD1	3:G:10:ASP:N	2.46	0.47
1:A:281:VAL:O	1:A:285:ASN:ND2	2.48	0.47
2:K:124:PRO:HA	2:K:149:ASN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:OG1	1:A:345:ARG:NH1	2.38	0.47
2:K:177:GLN:HB3	2:K:184:TYR:CZ	2.49	0.47
1:B:361:LYS:HB3	1:B:409:SER:HA	1.96	0.47
1:B:434:PHE:HB2	1:B:451:CYS:SG	2.55	0.47
3:D:91:THR:HG23	3:D:113:THR:HA	1.96	0.47
3:D:156:THR:HG23	3:D:199:ASN:HB2	1.97	0.47
3:H:127:LEU:HD21	3:H:144:LEU:HB2	1.97	0.46
2:C:151:TYR:HB3	2:C:209:HIS:CE1	2.50	0.46
3:G:151:GLU:N	3:G:152:PRO:HD2	2.31	0.46
3:D:3:GLN:HB2	3:D:25:THR:HB	1.95	0.46
1:A:328:GLY:HA3	1:A:400:PRO:HB3	1.97	0.46
2:L:15:VAL:HA	2:L:78:VAL:HG23	1.97	0.46
1:E:327:VAL:HG11	2:K:50:TRP:CZ2	2.51	0.46
1:E:249:LEU:HD21	1:E:515:PHE:HZ	1.80	0.46
1:A:323:THR:HG21	1:A:360:PRO:HG3	1.98	0.46
1:A:484:ARG:NE	1:B:523:GLN:HG3	2.31	0.46
3:H:149:PHE:HB2	3:H:177:LEU:HD22	1.98	0.46
1:E:361:LYS:HB3	1:E:409:SER:HA	1.98	0.46
1:E:475:LEU:HD11	1:E:491:LEU:HD22	1.97	0.46
2:C:204:THR:HG21	2:C:217:VAL:HG13	1.98	0.46
2:K:35:TRP:CE2	2:K:73:LEU:HB2	2.51	0.46
3:G:145:VAL:HG13	3:G:180:LEU:HB3	1.98	0.46
2:L:151:TYR:HB3	2:L:152:PRO:HD3	1.98	0.45
1:B:275:THR:HG22	1:B:322:GLY:H	1.81	0.45
2:C:16:GLY:HA2	2:C:77:ASN:HA	1.97	0.45
2:C:161:ILE:HG13	2:C:161:ILE:O	2.16	0.45
3:D:12:VAL:HG21	3:D:18:LEU:HD11	1.99	0.45
1:E:282:ASN:HA	1:E:285:ASN:ND2	2.31	0.45
1:E:432:LEU:HB2	1:E:499:VAL:HG13	1.99	0.45
3:H:29:ILE:HD11	3:H:74:THR:HA	1.97	0.45
1:B:395:THR:O	1:B:398:ASN:ND2	2.25	0.45
2:L:119:ARG:HG2	2:L:120:ALA:N	2.31	0.45
2:L:155:ILE:HG23	2:L:186:MET:HE3	1.98	0.45
3:H:51:TYR:CE2	3:H:59:ASN:HB3	2.51	0.45
1:B:303:LEU:HD23	1:B:320:PRO:HG2	1.99	0.45
1:E:431:LEU:HD23	1:E:498:THR:HG22	1.99	0.45
2:L:174:TRP:HD1	2:L:186:MET:HB2	1.81	0.45
2:C:196:GLU:HA	2:C:199:ARG:HG2	1.98	0.44
1:E:242:PHE:O	1:E:244:ILE:N	2.47	0.44
3:H:202:HIS:CG	3:H:203:PRO:HD2	2.52	0.44
2:C:129:PHE:HE2	2:C:146:PHE:HD2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:41:PHE:N	3:G:45:LYS:O	2.43	0.44
1:B:249:LEU:HB2	1:B:507:LEU:HB2	1.99	0.44
2:K:127:SER:HB3	2:K:129:PHE:CZ	2.53	0.44
3:G:36:HIS:ND1	3:G:51:TYR:HB3	2.33	0.44
2:L:107:LYS:HB3	2:L:114:LYS:HE2	2.00	0.44
1:E:321:LEU:HD12	1:E:321:LEU:H	1.83	0.44
2:K:174:TRP:CD1	2:K:186:MET:HB2	2.51	0.44
1:A:434:PHE:HB2	1:A:451:CYS:SG	2.57	0.44
2:K:114:LYS:HD2	2:K:151:TYR:HE1	1.82	0.44
3:D:147:GLY:HA2	3:D:177:LEU:HG	1.99	0.44
2:K:128:ILE:HG12	2:K:145:CYS:SG	2.58	0.44
3:H:186:VAL:HG22	3:H:188:SER:H	1.82	0.44
2:C:126:VAL:HG22	2:C:147:LEU:HG	2.00	0.44
1:E:282:ASN:HA	1:E:285:ASN:HD22	1.83	0.44
2:C:207:ALA:HB3	2:C:216:ILE:HB	1.99	0.43
1:E:320:PRO:HD2	1:E:360:PRO:HB2	2.00	0.43
2:K:151:TYR:CD1	2:K:152:PRO:HD2	2.53	0.43
1:A:356:ALA:HB2	1:A:411:ARG:HD2	2.00	0.43
3:H:12:VAL:HG21	3:H:18:LEU:HD11	2.00	0.43
1:B:426:PHE:CE2	1:B:524:PHE:HA	2.53	0.43
2:K:23:CYS:HB3	2:K:71:PHE:HB2	2.00	0.43
1:A:336:GLN:NE2	1:A:376:GLU:O	2.34	0.43
2:C:66:GLY:HA3	2:C:71:PHE:HA	2.00	0.43
3:D:100:VAL:HG12	3:D:104:GLU:HG3	1.99	0.43
1:E:334:LEU:HD21	1:E:367:PHE:CD2	2.53	0.43
2:K:152:PRO:HD3	2:K:184:TYR:CD1	2.54	0.43
1:A:293:ILE:HG21	3:H:54:TYR:CD1	2.53	0.43
2:L:34:ALA:HB2	2:L:91:TYR:OH	2.19	0.43
1:B:470:SER:HB2	1:B:522:ASN:HB2	1.99	0.43
2:C:166:ARG:HH22	2:C:192:LEU:HD22	1.82	0.43
3:D:164:SER:HG	3:D:185:THR:H	1.65	0.43
2:K:114:LYS:HD2	2:K:151:TYR:CE1	2.53	0.43
1:A:293:ILE:HG21	3:H:54:TYR:HD1	1.84	0.43
2:K:15:VAL:HA	2:K:78:VAL:O	2.19	0.43
3:H:38:ILE:HD11	3:H:103:PHE:HE2	1.84	0.43
2:C:50:TRP:C	2:C:52:SER:H	2.26	0.43
2:K:152:PRO:HD3	2:K:184:TYR:CG	2.53	0.43
1:B:414:HIS:HB2	2:C:93:ILE:HD11	2.00	0.43
3:H:36:HIS:ND1	3:H:51:TYR:HB3	2.33	0.42
1:B:232:LEU:HD22	1:B:456:GLU:HG2	2.00	0.42
2:K:12:SER:HA	2:K:104:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:178:ASP:HB2	2:C:182:SER:N	2.26	0.42
3:H:60:TYR:HE1	3:H:70:ILE:HG13	1.84	0.42
2:C:34:ALA:HB2	2:C:91:TYR:OH	2.19	0.42
2:C:35:TRP:CE2	2:C:73:LEU:HB2	2.54	0.42
2:K:151:TYR:HB3	2:K:153:LYS:HE3	2.01	0.42
1:A:242:PHE:O	1:A:244:ILE:N	2.52	0.42
2:L:171:LEU:HB3	3:H:172:VAL:HG21	2.02	0.42
1:E:357:ASP:HB3	1:E:366:GLN:CG	2.49	0.42
1:B:311:TYR:CE1	1:B:320:PRO:HG3	2.55	0.42
1:E:242:PHE:HD2	1:E:244:ILE:HD12	1.85	0.42
3:G:122:PRO:HG3	3:G:202:HIS:HB2	2.01	0.42
2:C:29:VAL:HG22	2:C:32:ALA:HB3	2.00	0.42
2:L:89:GLN:HA	2:L:97:THR:O	2.20	0.42
1:A:266:CYS:HB2	1:A:458:VAL:HG13	2.02	0.42
1:A:320:PRO:HD2	1:A:360:PRO:HB2	2.01	0.42
2:L:79:GLN:NE2	2:L:81:GLU:OE2	2.53	0.42
2:L:152:PRO:HD2	2:L:209:HIS:CE1	2.55	0.42
2:C:166:ARG:NE	2:C:190:LEU:HD22	2.35	0.42
3:D:23:THR:HA	3:D:78:GLN:HG2	2.01	0.42
1:B:411:ARG:NH2	2:C:96:TYR:OH	2.53	0.41
2:C:37:GLN:HB2	2:C:47:LEU:HD11	2.02	0.41
2:L:181:ASP:OD1	2:L:181:ASP:N	2.49	0.41
3:D:83:LEU:HD22	3:D:86:VAL:HG12	2.02	0.41
2:K:47:LEU:HD21	2:K:62:PHE:CD1	2.55	0.41
3:H:83:LEU:HD22	3:H:86:VAL:HG22	2.01	0.41
2:C:29:VAL:HG23	2:C:92:SER:HB3	2.02	0.41
2:K:122:ALA:O	2:K:209:HIS:NE2	2.53	0.41
2:K:147:LEU:HB2	2:K:186:MET:HG2	2.02	0.41
1:A:284:CYS:HB2	1:A:385:PRO:HG3	2.01	0.41
1:A:415:ASN:HB3	1:A:418:LEU:HD21	2.03	0.41
2:K:89:GLN:HB3	2:K:98:PHE:CE1	2.56	0.41
3:G:18:LEU:CD1	3:G:86:VAL:HG11	2.49	0.41
1:E:285:ASN:OD1	1:E:385:PRO:HD2	2.20	0.41
1:A:507:LEU:HG	1:A:530:MET:HE2	2.03	0.41
2:C:175:THR:HG22	2:C:185:SER:O	2.20	0.41
1:E:234:VAL:HG21	1:E:249:LEU:HD11	2.03	0.41
1:A:278:LEU:H	1:A:278:LEU:HD12	1.86	0.41
3:H:162:LEU:HD23	3:H:162:LEU:H	1.85	0.41
2:C:119:ARG:NH2	2:C:150:PHE:O	2.54	0.41
1:A:275:THR:HG21	1:A:319:ALA:HB3	2.02	0.41
1:E:347:HIS:HD2	1:E:371:THR:HG21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:50:TRP:C	2:L:52:SER:H	2.29	0.40
2:L:200:HIS:HB2	2:L:203:TYR:OH	2.21	0.40
1:B:230:PRO:HB2	1:B:232:LEU:HD13	2.02	0.40
1:E:249:LEU:HD23	1:E:432:LEU:HD21	2.03	0.40
3:D:21:THR:HG23	3:D:80:PHE:HE1	1.85	0.40
2:L:174:TRP:CD1	2:L:186:MET:HB2	2.55	0.40
3:H:122:PRO:HB3	3:H:148:TYR:HB3	2.04	0.40
3:D:48:TRP:CZ2	3:D:50:GLY:HA2	2.56	0.40
1:E:237:MET:HE3	1:E:246:LEU:HD12	2.03	0.40
3:G:78:GLN:HB3	3:G:80:PHE:CE1	2.57	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	305/311 (98%)	287 (94%)	18 (6%)	0	100	100
1	B	305/311 (98%)	285 (93%)	20 (7%)	0	100	100
1	E	305/311 (98%)	294 (96%)	11 (4%)	0	100	100
2	C	209/225 (93%)	192 (92%)	17 (8%)	0	100	100
2	K	161/225 (72%)	140 (87%)	21 (13%)	0	100	100
2	L	211/225 (94%)	192 (91%)	19 (9%)	0	100	100
3	D	196/224 (88%)	180 (92%)	16 (8%)	0	100	100
3	G	172/224 (77%)	150 (87%)	22 (13%)	0	100	100
3	H	204/224 (91%)	188 (92%)	16 (8%)	0	100	100
All	All	2068/2280 (91%)	1908 (92%)	160 (8%)	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	268/271 (99%)	268 (100%)	0	100	100
1	B	268/271 (99%)	268 (100%)	0	100	100
1	E	268/271 (99%)	268 (100%)	0	100	100
2	C	187/196 (95%)	187 (100%)	0	100	100
2	K	149/196 (76%)	149 (100%)	0	100	100
2	L	189/196 (96%)	189 (100%)	0	100	100
3	D	180/202 (89%)	180 (100%)	0	100	100
3	G	162/202 (80%)	162 (100%)	0	100	100
3	H	186/202 (92%)	186 (100%)	0	100	100
All	All	1857/2007 (92%)	1857 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	455	GLN
1	A	469	GLN
1	A	505	HIS
3	H	78	GLN
2	C	90	GLN
3	D	16	GLN
1	E	501	HIS

### 5.3.3 RNA ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	307/311 (98%)	0.09	5 (1%) 70 55	54, 87, 121, 172	0
1	B	307/311 (98%)	0.19	9 (2%) 53 39	45, 81, 117, 154	0
1	E	307/311 (98%)	0.32	7 (2%) 61 45	58, 101, 143, 168	0
2	C	213/225 (94%)	0.66	19 (8%) 15 13	69, 123, 172, 212	0
2	K	173/225 (76%)	1.12	37 (21%) 2 4	80, 125, 171, 182	0
2	L	215/225 (95%)	0.50	16 (7%) 20 16	61, 114, 162, 206	0
3	D	202/224 (90%)	0.50	16 (7%) 18 15	64, 101, 156, 181	0
3	G	180/224 (80%)	0.80	20 (11%) 10 10	80, 121, 161, 176	0
3	H	208/224 (92%)	0.39	8 (3%) 44 31	59, 93, 160, 173	0
All	All	2112/2280 (92%)	0.45	137 (6%) 25 18	45, 101, 158, 212	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	94	TYR	5.2
2	K	105	GLU	4.7
3	H	33	TYR	4.7
2	L	182	SER	4.4
2	K	114	LYS	4.3
2	C	83	LEU	4.3
2	K	111	GLY	4.1
2	K	217	VAL	4.0
3	H	188	SER	3.9
3	D	210	ASP	3.9
2	K	152	PRO	3.8
3	D	133	ALA	3.8
2	K	95	PRO	3.7
2	K	113	THR	3.7
3	H	210	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	L	106	ILE	3.6
2	K	218	LYS	3.4
3	G	18	LEU	3.4
2	K	182	SER	3.4
3	G	127	LEU	3.4
2	K	92	SER	3.4
3	D	166	VAL	3.3
2	K	93	ILE	3.3
2	K	146	PHE	3.3
2	C	166	ARG	3.2
2	K	207	ALA	3.2
2	K	120	ALA	3.2
1	E	321	LEU	3.2
3	G	186	VAL	3.2
3	G	198	CYS	3.1
2	K	106	ILE	3.1
2	C	146	PHE	3.0
1	E	530	MET	3.0
1	B	374	ASP	3.0
2	K	186	MET	3.0
3	G	125	TYR	3.0
2	C	62	PHE	3.0
3	G	33	TYR	3.0
2	K	183	THR	2.9
2	K	151	TYR	2.9
3	D	151	GLU	2.9
2	C	104	LEU	2.9
1	B	354	GLY	2.9
2	C	2	ILE	2.8
2	K	2	ILE	2.8
1	A	440	GLY	2.8
2	K	96	TYR	2.8
2	K	145	CYS	2.8
1	E	322	GLY	2.8
3	G	113	THR	2.8
1	A	530	MET	2.7
2	K	184	TYR	2.7
3	G	19	SER	2.7
2	C	91	TYR	2.7
3	D	192	PRO	2.7
1	B	447	MET	2.7
2	L	105	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	G	182	SER	2.7
3	H	190	PRO	2.7
1	B	459	GLN	2.7
1	B	375	PHE	2.7
2	C	144	VAL	2.7
2	C	191	THR	2.6
2	C	105	GLU	2.6
2	C	205	CYS	2.6
2	C	197	TYR	2.6
3	H	34	SER	2.6
1	B	277	GLN	2.6
3	H	173	LEU	2.6
1	B	376	GLU	2.6
3	D	168	THR	2.6
3	G	30	THR	2.5
2	C	115	LEU	2.5
3	G	181	SER	2.5
3	G	2	VAL	2.5
2	K	97	THR	2.5
3	D	132	ALA	2.5
2	C	186	MET	2.5
2	K	177	GLN	2.5
2	L	114	LYS	2.4
2	K	159	TRP	2.4
3	D	28	SER	2.4
2	K	104	LEU	2.4
2	L	2	ILE	2.4
1	A	355	SER	2.4
3	G	160	GLY	2.4
1	E	407	SER	2.4
3	D	165	GLY	2.4
2	K	90	GLN	2.4
2	C	221	ASN	2.3
2	L	90	GLN	2.3
2	L	92	SER	2.3
2	K	103	LYS	2.3
1	E	277	GLN	2.3
3	G	55	SER	2.3
2	C	107	LYS	2.3
3	D	203	PRO	2.3
2	L	99	GLY	2.3
2	L	191	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	G	115	SER	2.3
2	K	47	LEU	2.3
3	G	184	VAL	2.3
2	C	99	GLY	2.3
2	L	168	ASN	2.3
2	K	107	LYS	2.2
3	G	178	TYR	2.2
2	C	155	ILE	2.2
2	L	107	LYS	2.2
2	K	5	THR	2.2
3	D	162	LEU	2.2
3	G	168	THR	2.2
3	D	55	SER	2.2
3	D	163	SER	2.2
2	L	104	LEU	2.2
2	L	117	ILE	2.2
3	D	201	ALA	2.2
1	B	264	GLY	2.1
2	K	211	THR	2.1
2	L	161	ILE	2.1
1	E	264	GLY	2.1
3	D	169	PHE	2.1
3	G	169	PHE	2.1
3	G	144	LEU	2.1
1	A	354	GLY	2.1
2	L	169	GLY	2.1
2	L	160	LYS	2.1
1	A	273	LEU	2.1
3	H	129	PRO	2.1
2	K	27	GLN	2.1
3	D	150	PRO	2.1
2	K	128	ILE	2.0
1	E	333	MET	2.0
2	C	181	ASP	2.0
1	B	348	LYS	2.0
2	K	187	SER	2.0
2	K	15	VAL	2.0
3	H	2	VAL	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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.