



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2016 – 10:03 PM EDT

PDB ID : 5AAW  
Title : Structure of a redesigned cross-reactive antibody to dengue virus with increased in vivo potency  
Authors : Wong, Y.; Robinson, L.; Lescar, J.; Sasisekharan, R.  
Deposited on : 2015-07-30  
Resolution : 3.27 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  
<http://wwpdb.org/validation/2016/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  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

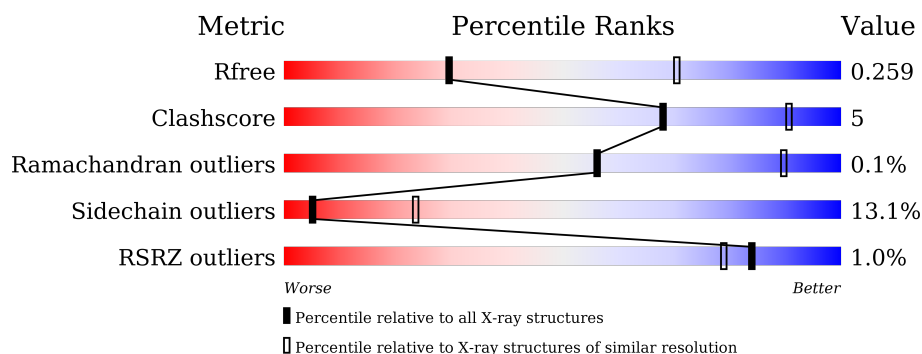
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.27 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))
$R_{free}$	91344	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	252	<div> <div>73%</div> <div>14%</div> <div>•</div> <div>10%</div> </div>
1	B	252	<div> <div>%</div> <div>72%</div> <div>17%</div> <div>•</div> <div>9%</div> </div>
1	D	252	<div> <div>75%</div> <div>13%</div> <div>•</div> <div>10%</div> </div>
1	F	252	<div> <div>69%</div> <div>15%</div> <div>6%</div> <div>10%</div> </div>
1	H	252	<div> <div>73%</div> <div>15%</div> <div>•</div> <div>10%</div> </div>
1	K	252	<div> <div>71%</div> <div>17%</div> <div>•</div> <div>10%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	115	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>62%</div><div>19%</div><div>•</div><div>17%</div></div></div>
2	E	115	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>71%</div><div>12%</div><div></div><div>17%</div></div></div>
2	G	115	<div><div><div></div><div></div><div></div></div><div><div>9%</div><div>65%</div><div>15%</div><div>•</div><div>19%</div></div></div>
2	I	115	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>70%</div><div>13%</div><div>•</div><div>17%</div></div></div>
2	J	115	<div><div><div></div><div></div><div></div></div><div><div></div><div>72%</div><div>10%</div><div>•</div><div>17%</div></div></div>
2	L	115	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>71%</div><div>11%</div><div>•</div><div>17%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15132 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 SCFV513.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1779	1116	307	346	10			
1	B	229	Total	C	N	O	S	0	0	0
			1788	1121	309	348	10			
1	D	228	Total	C	N	O	S	0	0	0
			1779	1116	307	346	10			
1	F	227	Total	C	N	O	S	0	0	0
			1773	1113	306	344	10			
1	H	228	Total	C	N	O	S	0	1	0
			1787	1122	308	347	10			
1	K	228	Total	C	N	O	S	0	0	0
			1779	1116	307	346	10			

- Molecule 2 is a protein called DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	96	Total	C	N	O	S	0	1	0
			745	471	126	144	4			
2	E	96	Total	C	N	O	S	0	0	0
			737	467	124	142	4			
2	G	93	Total	C	N	O	S	0	0	0
			706	446	117	139	4			
2	I	96	Total	C	N	O	S	0	0	0
			737	467	124	142	4			
2	J	96	Total	C	N	O	S	0	0	0
			737	467	124	142	4			
2	L	96	Total	C	N	O	S	0	1	0
			745	471	126	144	4			

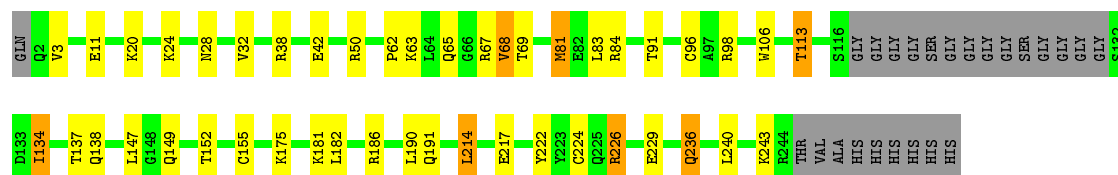
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	6	Total O 6 6	0	0
3	C	2	Total O 2 2	0	0
3	D	4	Total O 4 4	0	0
3	E	5	Total O 5 5	0	0
3	F	5	Total O 5 5	0	0
3	G	4	Total O 4 4	0	0
3	H	3	Total O 3 3	0	0
3	J	3	Total O 3 3	0	0
3	K	1	Total O 1 1	0	0
3	L	4	Total O 4 4	0	0



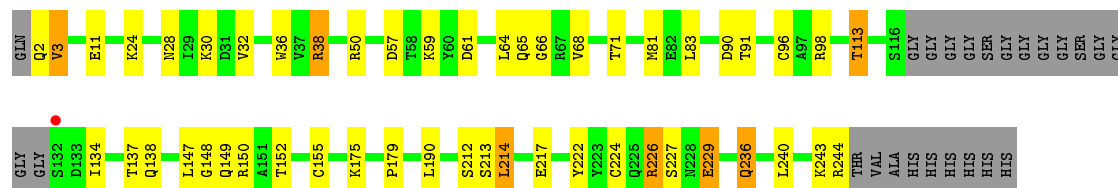
- Molecule 1: SCFV513

Chain H:  73% 15% 10%



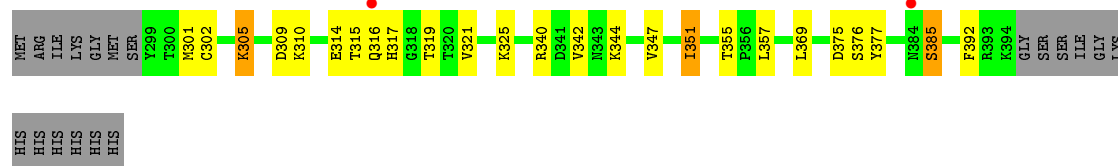
- Molecule 1: SCFV513

Chain K:  71% 17% 10%



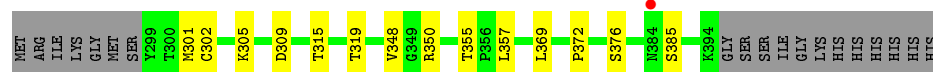
- Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain C: 



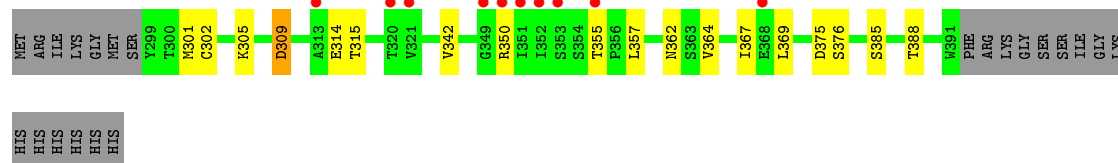
- Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain E:  %



- Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain G:  9% 65% 15% 19%



- Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

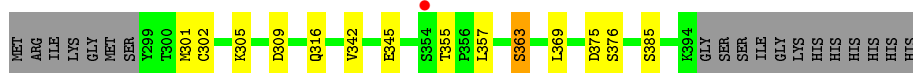
Chain I:  %

- Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain J:  72% 10% • 17%

- Molecule 2: DENGUE SEROTYPE 4 ENVELOPE PROTEIN DOMAIN 3

Chain L: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.11Å 131.67Å 176.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 3.27 45.71 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.75-3.27) 99.8 (45.71-3.27)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.227 , 0.263 0.225 , 0.259	Depositor DCC
$R_{free}$ test set	1618 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 31.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	4 of 31967 reflections (0.013%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	15132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.53	0/1819	0.74	1/2465 (0.0%)
1	B	0.49	0/1828	0.71	1/2477 (0.0%)
1	D	0.52	0/1819	0.74	1/2465 (0.0%)
1	F	0.59	0/1813	0.85	3/2457 (0.1%)
1	H	0.52	0/1827	0.74	0/2476
1	K	0.53	0/1819	0.77	2/2465 (0.1%)
2	C	0.54	0/759	0.80	1/1028 (0.1%)
2	E	0.51	0/751	0.74	0/1017
2	G	0.58	0/719	0.81	0/976
2	I	0.52	0/751	0.76	0/1017
2	J	0.51	0/751	0.75	0/1017
2	L	0.51	0/759	0.83	1/1028 (0.1%)
All	All	0.53	0/15415	0.77	10/20888 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	31	ASP	CB-CG-OD1	9.29	126.66	118.30
2	C	302	CYS	CA-CB-SG	7.82	128.07	114.00
1	K	227	SER	CB-CA-C	-7.60	95.65	110.10
1	F	31	ASP	CB-CG-OD2	-7.29	111.73	118.30
1	D	133	ASP	CB-CG-OD1	5.55	123.29	118.30
2	L	363	SER	CB-CA-C	-5.53	99.60	110.10
1	B	84	ARG	CG-CD-NE	-5.52	100.22	111.80
1	K	61	ASP	CB-CG-OD1	5.49	123.24	118.30
1	F	87	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	162	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1779	0	1718	18	0
1	B	1788	0	1729	19	0
1	D	1779	0	1718	12	0
1	F	1773	0	1713	25	0
1	H	1787	0	1728	28	0
1	K	1779	0	1718	13	0
2	C	745	0	746	22	0
2	E	737	0	741	4	0
2	G	706	0	706	5	0
2	I	737	0	741	5	0
2	J	737	0	741	3	0
2	L	745	0	746	11	0
3	A	3	0	0	0	0
3	B	6	0	0	0	0
3	C	2	0	0	0	0
3	D	4	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	4	0	0	0	0
3	H	3	0	0	0	0
3	J	3	0	0	1	0
3	K	1	0	0	0	0
3	L	4	0	0	0	0
All	All	15132	0	14745	140	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 5.

All (140) 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:H:182[B]:LEU:HD23	1:H:182[B]:LEU:H	1.14	1.05
1:H:68:VAL:HG12	1:H:81:MET:CE	1.85	1.05
2:C:316:GLN:HB2	2:L:316:GLN:HB3	1.43	0.97
1:H:138:GLN:H	1:H:236:GLN:HE22	1.15	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:GLN:H	1:F:236:GLN:HE22	1.16	0.92
1:B:138:GLN:H	1:B:236:GLN:HE22	1.16	0.90
1:A:138:GLN:H	1:A:236:GLN:HE22	1.15	0.89
1:K:138:GLN:H	1:K:236:GLN:HE22	1.16	0.88
2:G:305:LYS:HG2	2:G:385:SER:HB2	1.55	0.86
1:H:182[B]:LEU:CD2	1:H:182[B]:LEU:H	1.78	0.81
1:H:182[B]:LEU:HD23	1:H:182[B]:LEU:N	1.98	0.78
1:H:68:VAL:HG12	1:H:81:MET:HE3	1.65	0.78
1:F:17:ALA:O	1:F:86:LEU:HD13	1.84	0.77
2:C:316:GLN:CB	2:L:316:GLN:HB3	2.15	0.76
2:J:299:TYR:N	3:J:2001:HOH:O	2.24	0.71
1:H:181:LYS:HD3	1:H:182[B]:LEU:HG	1.74	0.70
1:D:39:GLN:NE2	1:D:174:GLN:HE22	1.91	0.69
1:K:65:GLN:HE21	1:K:66:GLY:H	1.41	0.69
1:F:15:PRO:HD3	1:F:115:SER:O	1.93	0.68
1:K:148:GLY:O	1:K:213:SER:HB2	1.93	0.67
2:C:351:ILE:HD13	2:C:351:ILE:H	1.59	0.67
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.30	0.65
2:C:315:THR:CG2	2:C:321:VAL:HG23	2.27	0.65
1:D:39:GLN:HE22	1:D:174:GLN:HE22	1.46	0.64
2:C:315:THR:O	2:L:316:GLN:HG2	1.97	0.64
1:B:73:ASP:OD2	1:H:69:THR:HG23	1.98	0.63
1:H:182[B]:LEU:HD12	1:H:191:GLN:HG2	1.81	0.62
1:B:20:LYS:HD3	1:H:20:LYS:HD3	1.81	0.61
1:H:68:VAL:HG12	1:H:81:MET:HE1	1.75	0.61
1:F:32:VAL:HG23	2:G:309:ASP:OD1	2.01	0.59
1:A:134:ILE:HD13	1:A:226:ARG:CZ	2.32	0.59
1:H:68:VAL:CG1	1:H:81:MET:HE3	2.32	0.59
1:F:134:ILE:HG23	1:F:159:GLU:HG3	1.86	0.57
2:E:305:LYS:HE2	2:E:385:SER:HB3	1.87	0.57
1:F:86:LEU:HB3	1:F:114:VAL:HG11	1.86	0.57
1:F:55:ASN:OD1	1:F:57:ASP:HB2	2.05	0.56
1:F:243:LYS:HD3	1:F:244:ARG:HG3	1.87	0.56
1:F:31:ASP:HB3	2:G:364:VAL:HG21	1.88	0.56
2:C:342:VAL:HG12	2:C:375:ASP:HB2	1.87	0.55
2:C:316:GLN:CD	2:L:316:GLN:O	2.45	0.55
2:C:375:ASP:OD1	2:C:392:PHE:HD1	1.89	0.55
1:K:226:ARG:NH1	1:K:229:GLU:O	2.40	0.55
2:I:305:LYS:HE2	2:I:385:SER:HB3	1.88	0.54
2:J:371:PRO:O	2:J:393:ARG:NH1	2.41	0.54
1:H:182[B]:LEU:N	1:H:182[B]:LEU:CD2	2.57	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HD21	1:A:240:LEU:HD21	1.91	0.53
1:F:214:LEU:HD21	1:F:240:LEU:HD21	1.91	0.53
1:H:214:LEU:HD21	1:H:240:LEU:HD21	1.91	0.53
1:F:64:LEU:HD12	1:F:68:VAL:HG21	1.91	0.53
1:K:214:LEU:HD21	1:K:240:LEU:HD21	1.91	0.53
1:B:214:LEU:HD21	1:B:240:LEU:HD21	1.91	0.53
1:B:226:ARG:NH1	1:B:229:GLU:O	2.42	0.52
1:K:138:GLN:NE2	1:K:222:TYR:O	2.42	0.52
1:D:214:LEU:HD21	1:D:240:LEU:HD21	1.91	0.52
1:A:91:THR:HG23	1:A:113:THR:HA	1.92	0.51
1:F:32:VAL:HG21	1:F:98:ARG:NE	2.25	0.51
2:E:348:VAL:HG21	2:E:372:PRO:HG3	1.92	0.51
1:K:91:THR:HG23	1:K:113:THR:HA	1.92	0.51
1:H:138:GLN:NE2	1:H:222:TYR:O	2.43	0.51
1:D:138:GLN:NE2	1:D:222:TYR:O	2.44	0.51
1:B:91:THR:HG23	1:B:113:THR:HA	1.93	0.50
2:E:315:THR:CG2	2:E:319:THR:OG1	2.59	0.50
1:H:91:THR:HG23	1:H:113:THR:HA	1.92	0.50
1:B:138:GLN:NE2	1:B:222:TYR:O	2.44	0.50
2:J:355:THR:HG22	2:J:355:THR:O	2.12	0.50
1:B:175:LYS:HE2	1:B:217:GLU:O	2.12	0.49
1:F:91:THR:HG23	1:F:113:THR:HA	1.94	0.49
2:I:341:ASP:HB2	2:I:346:LYS:HB3	1.95	0.49
1:F:138:GLN:NE2	1:F:222:TYR:O	2.46	0.49
1:K:175:LYS:HE2	1:K:217:GLU:O	2.11	0.49
2:L:355:THR:O	2:L:355:THR:HG22	2.12	0.49
1:A:138:GLN:NE2	1:A:222:TYR:O	2.45	0.49
1:H:175:LYS:HE2	1:H:217:GLU:O	2.12	0.49
1:A:87:ARG:NH1	1:B:87:ARG:NH2	2.61	0.49
1:D:91:THR:HG23	1:D:113:THR:HA	1.93	0.49
1:F:175:LYS:HE2	1:F:217:GLU:O	2.11	0.49
1:A:175:LYS:HE2	1:A:217:GLU:O	2.13	0.48
1:F:15:PRO:HB2	1:H:62:PRO:HB3	1.95	0.48
1:H:182[B]:LEU:O	1:H:182[B]:LEU:HG	2.13	0.48
2:C:316:GLN:HB2	2:L:316:GLN:O	2.13	0.48
2:E:355:THR:HG22	2:E:355:THR:O	2.13	0.48
1:H:226:ARG:NH1	1:H:229:GLU:O	2.47	0.47
1:D:175:LYS:HE2	1:D:217:GLU:O	2.13	0.47
2:C:317:HIS:NE2	2:L:316:GLN:NE2	2.62	0.47
2:L:363:SER:O	2:L:363:SER:OG	2.29	0.47
1:A:134:ILE:HD13	1:A:226:ARG:NH1	2.30	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:O	1:B:205:THR:HG23	2.14	0.47
1:A:105:TYR:HE2	2:C:325:LYS:HE3	1.80	0.47
1:B:3:VAL:HA	1:B:106:TRP:O	2.15	0.47
1:H:186:ARG:NH2	2:I:306:PHE:O	2.48	0.46
2:C:315:THR:O	2:L:316:GLN:CG	2.62	0.46
1:H:3:VAL:HA	1:H:106:TRP:O	2.15	0.46
1:A:67:ARG:HH22	1:A:90:ASP:CG	2.19	0.46
2:C:315:THR:OG1	2:C:319:THR:OG1	2.23	0.46
2:L:305:LYS:HE2	2:L:385:SER:HB2	1.96	0.46
1:D:226:ARG:NH1	1:D:229:GLU:O	2.48	0.46
2:I:355:THR:HG22	2:I:355:THR:O	2.15	0.46
1:F:4:GLN:O	1:F:25:ALA:HA	2.16	0.46
2:C:355:THR:O	2:C:355:THR:HG22	2.15	0.46
1:B:178:GLN:NE2	1:D:178:GLN:OE1	2.48	0.46
1:F:226:ARG:NH1	1:F:229:GLU:O	2.49	0.45
1:D:39:GLN:HE22	1:D:174:GLN:NE2	2.13	0.45
1:A:243:LYS:HE2	1:A:244:ARG:H	1.81	0.45
1:A:134:ILE:HD13	1:A:226:ARG:NH2	2.32	0.45
2:C:340:ARG:HG2	2:C:344:LYS:HA	1.98	0.45
1:A:87:ARG:NH1	1:B:87:ARG:HH22	2.15	0.44
1:A:30:LYS:O	2:C:310:LYS:NZ	2.51	0.44
1:A:20:LYS:NZ	1:K:71:THR:HG21	2.33	0.44
1:B:38:ARG:HH11	1:B:64:LEU:HD21	1.82	0.43
1:F:87:ARG:O	1:F:114:VAL:HG21	2.18	0.43
2:C:375:ASP:OD1	2:C:392:PHE:CD1	2.71	0.43
1:B:6:VAL:HG13	1:D:108:GLN:NE2	2.34	0.42
2:C:305:LYS:HG2	2:C:385:SER:HB2	2.00	0.42
1:B:216:ALA:HB2	1:D:242:ILE:HG13	2.00	0.42
1:D:3:VAL:HA	1:D:106:TRP:O	2.19	0.42
1:A:69:THR:OG1	1:A:84:ARG:NH2	2.46	0.42
2:C:340:ARG:HB3	2:C:377:TYR:HB2	2.02	0.42
1:H:181:LYS:HA	1:H:182[B]:LEU:HD23	2.02	0.42
1:K:3:VAL:HG11	1:K:179:PRO:HG2	2.02	0.42
2:C:375:ASP:OD1	2:C:375:ASP:N	2.53	0.42
1:F:134:ILE:HG12	1:F:226:ARG:CZ	2.50	0.42
1:F:166:ASN:ND2	2:G:388:THR:O	2.52	0.42
2:I:315:THR:CG2	2:I:321:VAL:HG23	2.49	0.41
2:G:342:VAL:HG13	2:G:375:ASP:HB2	2.02	0.41
1:A:38:ARG:HH12	1:A:90:ASP:HA	1.86	0.41
2:C:315:THR:HG22	2:C:321:VAL:HG23	1.99	0.41
1:F:47:TRP:CH2	1:F:49:GLY:HA2	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:36:TRP:CE2	1:K:81:MET:HB2	2.56	0.41
2:L:342:VAL:HG13	2:L:375:ASP:HB2	2.02	0.41
1:B:36:TRP:CE2	1:B:81:MET:HB2	2.56	0.41
1:F:87:ARG:HG2	1:H:63:LYS:HA	2.02	0.41
1:F:16:GLY:HA3	1:H:65:GLN:HB3	2.02	0.41
1:H:134:ILE:HG12	1:H:226:ARG:CZ	2.50	0.41
1:B:38:ARG:NH2	1:B:90:ASP:HA	2.35	0.40
1:B:47:TRP:CH2	1:B:49:GLY:HA2	2.56	0.40
1:F:15:PRO:CB	1:H:62:PRO:HB3	2.51	0.40
2:C:340:ARG:HH21	2:C:347:VAL:HG22	1.87	0.40
1:K:38:ARG:HH12	1:K:90:ASP:HA	1.86	0.40
1:H:67:ARG:HG2	1:H:84:ARG:O	2.22	0.40
1:K:57:ASP:OD1	1:K:59:LYS:HE2	2.22	0.40

There are no symmetry-related clashes.

## 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	A	224/252 (89%)	217 (97%)	7 (3%)	0	100	100
1	B	225/252 (89%)	217 (96%)	8 (4%)	0	100	100
1	D	224/252 (89%)	216 (96%)	8 (4%)	0	100	100
1	F	223/252 (88%)	216 (97%)	7 (3%)	0	100	100
1	H	225/252 (89%)	215 (96%)	10 (4%)	0	100	100
1	K	224/252 (89%)	216 (96%)	8 (4%)	0	100	100
2	C	95/115 (83%)	92 (97%)	3 (3%)	0	100	100
2	E	94/115 (82%)	91 (97%)	3 (3%)	0	100	100
2	G	91/115 (79%)	87 (96%)	4 (4%)	0	100	100
2	I	94/115 (82%)	90 (96%)	4 (4%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	94/115 (82%)	90 (96%)	3 (3%)	1 (1%)	17	59
2	L	95/115 (83%)	87 (92%)	8 (8%)	0	100	100
All	All	1908/2202 (87%)	1834 (96%)	73 (4%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	316	GLN

### 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	192/203 (95%)	164 (85%)	28 (15%)	4	19
1	B	193/203 (95%)	169 (88%)	24 (12%)	6	26
1	D	192/203 (95%)	168 (88%)	24 (12%)	6	26
1	F	191/203 (94%)	160 (84%)	31 (16%)	3	14
1	H	193/203 (95%)	168 (87%)	25 (13%)	5	24
1	K	192/203 (95%)	161 (84%)	31 (16%)	3	14
2	C	84/99 (85%)	75 (89%)	9 (11%)	8	33
2	E	83/99 (84%)	76 (92%)	7 (8%)	14	47
2	G	80/99 (81%)	68 (85%)	12 (15%)	3	17
2	I	83/99 (84%)	74 (89%)	9 (11%)	8	33
2	J	83/99 (84%)	74 (89%)	9 (11%)	8	33
2	L	84/99 (85%)	77 (92%)	7 (8%)	14	48
All	All	1650/1812 (91%)	1434 (87%)	216 (13%)	5	23

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	6	VAL
1	A	11	GLU
1	A	24	LYS
1	A	28	ASN
1	A	32	VAL
1	A	38	ARG
1	A	50	ARG
1	A	68	VAL
1	A	71	THR
1	A	83	LEU
1	A	84	ARG
1	A	96	CYS
1	A	98	ARG
1	A	113	THR
1	A	137	THR
1	A	147	LEU
1	A	149	GLN
1	A	152	THR
1	A	155	CYS
1	A	190	LEU
1	A	214	LEU
1	A	224	CYS
1	A	226	ARG
1	A	229	GLU
1	A	236	GLN
1	A	243	LYS
1	A	244	ARG
1	B	4	GLN
1	B	11	GLU
1	B	24	LYS
1	B	28	ASN
1	B	32	VAL
1	B	50	ARG
1	B	68	VAL
1	B	83	LEU
1	B	96	CYS
1	B	98	ARG
1	B	113	THR
1	B	134	ILE
1	B	137	THR
1	B	147	LEU
1	B	149	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	152	THR
1	B	155	CYS
1	B	190	LEU
1	B	214	LEU
1	B	224	CYS
1	B	226	ARG
1	B	229	GLU
1	B	236	GLN
1	B	243	LYS
2	C	301	MET
2	C	305	LYS
2	C	309	ASP
2	C	314	GLU
2	C	351	ILE
2	C	357	LEU
2	C	369	LEU
2	C	376	SER
2	C	385	SER
1	D	11	GLU
1	D	24	LYS
1	D	28	ASN
1	D	32	VAL
1	D	38	ARG
1	D	50	ARG
1	D	68	VAL
1	D	83	LEU
1	D	96	CYS
1	D	98	ARG
1	D	113	THR
1	D	134	ILE
1	D	137	THR
1	D	147	LEU
1	D	149	GLN
1	D	152	THR
1	D	155	CYS
1	D	190	LEU
1	D	214	LEU
1	D	224	CYS
1	D	226	ARG
1	D	229	GLU
1	D	236	GLN
1	D	243	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	301	MET
2	E	302	CYS
2	E	309	ASP
2	E	350	ARG
2	E	357	LEU
2	E	369	LEU
2	E	376	SER
1	F	2	GLN
1	F	11	GLU
1	F	24	LYS
1	F	32	VAL
1	F	38	ARG
1	F	50	ARG
1	F	64	LEU
1	F	68	VAL
1	F	71	THR
1	F	82	GLU
1	F	83	LEU
1	F	96	CYS
1	F	98	ARG
1	F	113	THR
1	F	114	VAL
1	F	134	ILE
1	F	137	THR
1	F	147	LEU
1	F	149	GLN
1	F	152	THR
1	F	155	CYS
1	F	190	LEU
1	F	197	ARG
1	F	212	SER
1	F	214	LEU
1	F	224	CYS
1	F	225	GLN
1	F	226	ARG
1	F	236	GLN
1	F	243	LYS
1	F	244	ARG
2	G	301	MET
2	G	302	CYS
2	G	309	ASP
2	G	314	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	315	THR
2	G	350	ARG
2	G	355	THR
2	G	357	LEU
2	G	362	ASN
2	G	367	ILE
2	G	369	LEU
2	G	376	SER
1	H	11	GLU
1	H	24	LYS
1	H	28	ASN
1	H	32	VAL
1	H	38	ARG
1	H	42	GLU
1	H	50	ARG
1	H	68	VAL
1	H	81	MET
1	H	83	LEU
1	H	96	CYS
1	H	98	ARG
1	H	113	THR
1	H	134	ILE
1	H	137	THR
1	H	147	LEU
1	H	149	GLN
1	H	152	THR
1	H	155	CYS
1	H	190	LEU
1	H	214	LEU
1	H	224	CYS
1	H	226	ARG
1	H	236	GLN
1	H	243	LYS
2	I	301	MET
2	I	302	CYS
2	I	309	ASP
2	I	317	HIS
2	I	341	ASP
2	I	357	LEU
2	I	369	LEU
2	I	376	SER
2	I	394	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	J	301	MET
2	J	302	CYS
2	J	309	ASP
2	J	310	LYS
2	J	316	GLN
2	J	344	LYS
2	J	357	LEU
2	J	369	LEU
2	J	376	SER
1	K	2	GLN
1	K	3	VAL
1	K	11	GLU
1	K	24	LYS
1	K	28	ASN
1	K	30	LYS
1	K	32	VAL
1	K	38	ARG
1	K	50	ARG
1	K	64	LEU
1	K	68	VAL
1	K	83	LEU
1	K	96	CYS
1	K	98	ARG
1	K	113	THR
1	K	134	ILE
1	K	137	THR
1	K	147	LEU
1	K	149	GLN
1	K	150	ARG
1	K	152	THR
1	K	155	CYS
1	K	190	LEU
1	K	212	SER
1	K	214	LEU
1	K	224	CYS
1	K	226	ARG
1	K	229	GLU
1	K	236	GLN
1	K	243	LYS
1	K	244	ARG
2	L	301	MET
2	L	302	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	309	ASP
2	L	345	GLU
2	L	357	LEU
2	L	369	LEU
2	L	376	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	B	236	GLN
2	C	384	ASN
1	D	4	GLN
1	D	39	GLN
2	E	384	ASN
1	F	225	GLN
1	F	236	GLN
1	H	236	GLN
2	I	384	ASN
2	J	384	ASN
2	J	390	HIS
1	K	65	GLN
1	K	236	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

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, 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	228/252 (90%)	-0.25	0 100 100	21, 39, 64, 83	1 (0%)
1	B	229/252 (90%)	-0.24	2 (0%) 85 81	22, 39, 74, 105	1 (0%)
1	D	228/252 (90%)	-0.18	1 (0%) 93 91	24, 41, 63, 92	1 (0%)
1	F	227/252 (90%)	-0.06	0 100 100	26, 47, 73, 95	1 (0%)
1	H	228/252 (90%)	-0.25	0 100 100	22, 40, 60, 81	1 (0%)
1	K	228/252 (90%)	-0.24	1 (0%) 93 91	22, 39, 64, 100	1 (0%)
2	C	96/115 (83%)	0.31	2 (2%) 67 58	38, 78, 107, 129	0
2	E	96/115 (83%)	0.03	1 (1%) 84 79	37, 58, 81, 93	0
2	G	93/115 (80%)	0.88	10 (10%) 8 5	63, 91, 124, 141	0
2	I	96/115 (83%)	0.22	1 (1%) 84 79	36, 73, 108, 119	0
2	J	96/115 (83%)	0.05	0 100 100	34, 61, 102, 122	0
2	L	96/115 (83%)	0.09	1 (1%) 84 79	38, 70, 93, 108	0
All	All	1941/2202 (88%)	-0.07	19 (0%) 84 79	21, 46, 95, 141	6 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	353	SER	5.7
2	G	349	GLY	4.3
2	G	313	ALA	3.7
1	B	132	SER	3.2
2	C	384	ASN	3.0
2	G	350	ARG	2.9
2	G	368	GLU	2.8
2	L	354	SER	2.6
2	G	321	VAL	2.6
1	D	132	SER	2.6
2	I	303	SER	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	G	320	THR	2.5
1	B	1	GLN	2.3
1	K	132	SER	2.3
2	C	316	GLN	2.2
2	G	351	ILE	2.1
2	E	384	ASN	2.1
2	G	352	ILE	2.0
2	G	355	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.