



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 12:28 PM EDT

PDB ID : 5KZP  
Title : Structure of the HCV1-C1 Antibody-Antigen Complex  
Authors : Piepenbrink, K.H.; Sundberg, E.J.  
Deposited on : 2016-07-25  
Resolution : 2.26 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

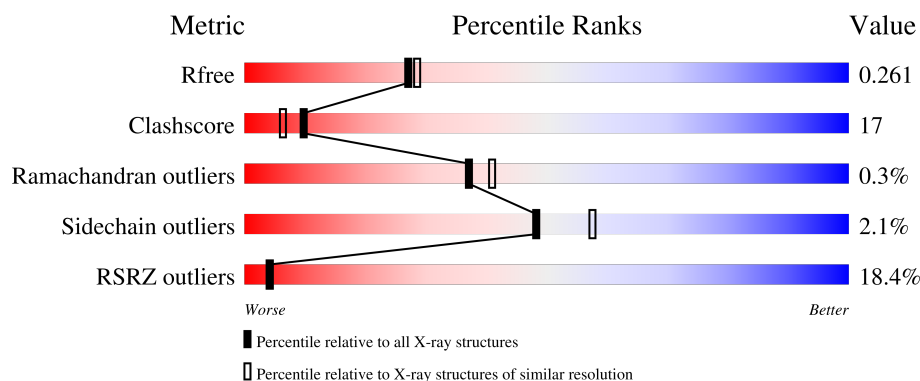
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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))
$R_{free}$	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	E	226	<div> <div>45%</div> <div>62%</div> <div>32%</div> <div>6%</div> </div>
1	F	226	<div> <div>20%</div> <div>82%</div> <div>17%</div> </div>
1	G	226	<div> <div>18%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>
1	H	226	<div> <div>6%</div> <div>84%</div> <div>16%</div> </div>
2	I	213	<div> <div>23%</div> <div>70%</div> <div>25%</div> <div>.</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	213	
2	K	213	
2	L	213	
3	A	15	
3	B	15	
3	C	15	
3	D	15	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	E	301	-	-	X	-
4	ACT	F	301	-	-	X	-
4	ACT	G	301	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14615 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 HCV1-C1 Antibody Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	226	Total	C	N	O	S	0	2	0
			1742	1109	291	334	8			
1	E	226	Total	C	N	O	S	0	1	0
			1727	1100	286	333	8			
1	F	226	Total	C	N	O	S	0	1	0
			1734	1103	290	333	8			
1	G	226	Total	C	N	O	S	0	1	0
			1733	1100	292	333	8			

- Molecule 2 is a protein called HCV1-C1 Antibody Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	3	0
			1658	1035	285	334	4			
2	I	212	Total	C	N	O	S	0	4	0
			1661	1039	284	334	4			
2	J	212	Total	C	N	O	S	0	4	0
			1660	1036	284	336	4			
2	K	211	Total	C	N	O	S	0	1	0
			1625	1014	278	329	4			

- Molecule 3 is a protein called C1 Epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	15	Total	C	N	O	S	0	0	0
			120	73	23	22	2			
3	B	15	Total	C	N	O	S	0	1	0
			125	76	24	23	2			
3	C	15	Total	C	N	O	S	0	1	0
			125	76	24	23	2			
3	D	15	Total	C	N	O	S	0	0	0
			120	73	23	22	2			

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Ca	0	0
			2	2		
5	L	2	Total	Ca	0	0
			2	2		
5	A	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		
5	F	4	Total	Ca	0	0
			4	4		
5	J	2	Total	Ca	0	0
			2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Ca 1	0	0
5	G	2	Total 2	Ca 2	0	0
5	K	5	Total 5	Ca 5	0	0

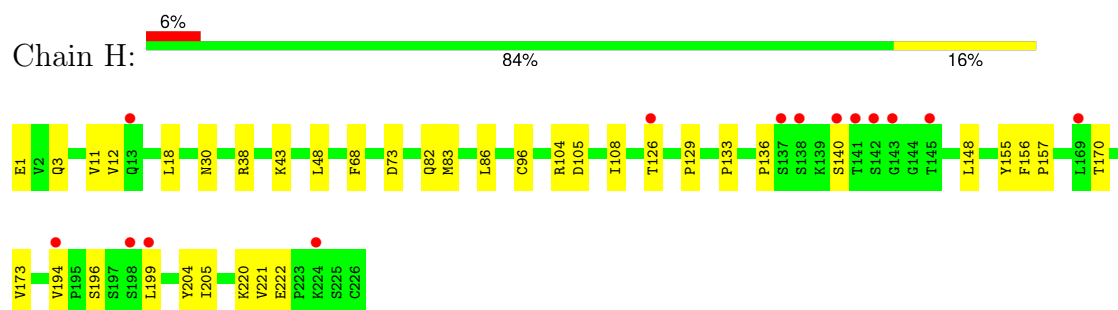
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	83	Total 83	O 83	0	0
6	L	85	Total 85	O 85	0	0
6	A	7	Total 7	O 7	0	0
6	E	48	Total 48	O 48	0	0
6	I	53	Total 53	O 53	0	0
6	B	10	Total 10	O 10	0	0
6	F	68	Total 68	O 68	0	0
6	J	76	Total 76	O 76	0	0
6	C	6	Total 6	O 6	0	0
6	G	60	Total 60	O 60	0	0
6	K	49	Total 49	O 49	0	0
6	D	3	Total 3	O 3	0	0

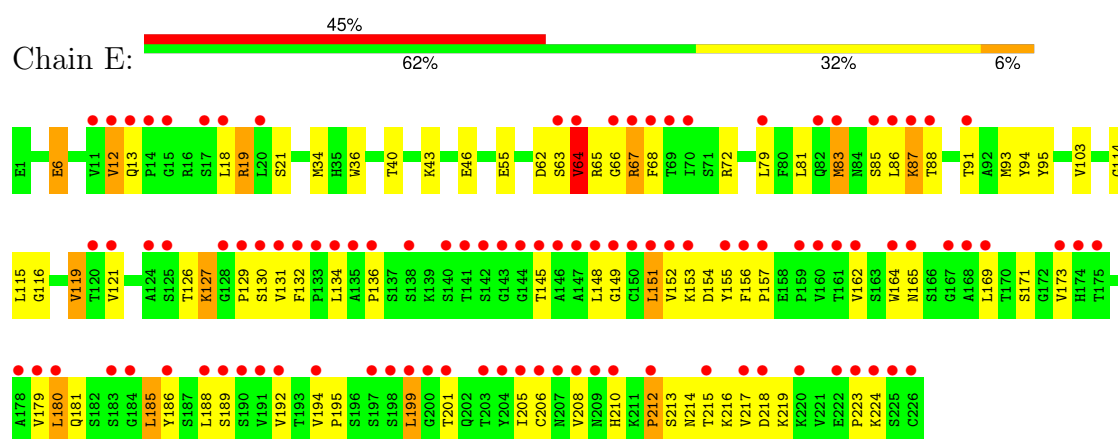
### 3 Residue-property plots [i](#)

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

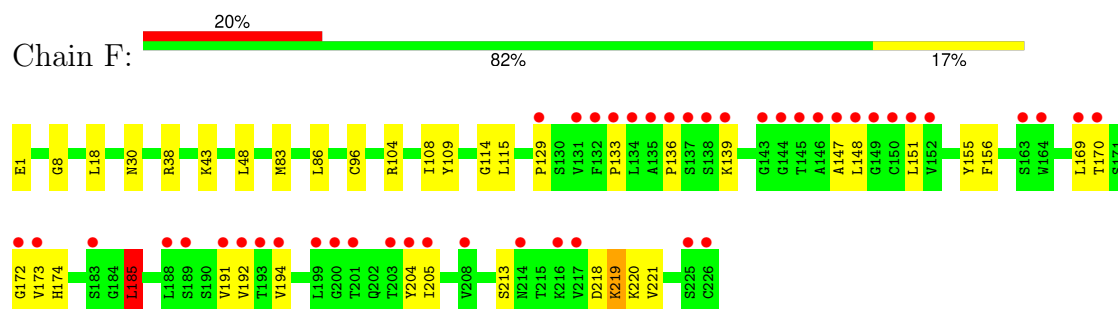
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



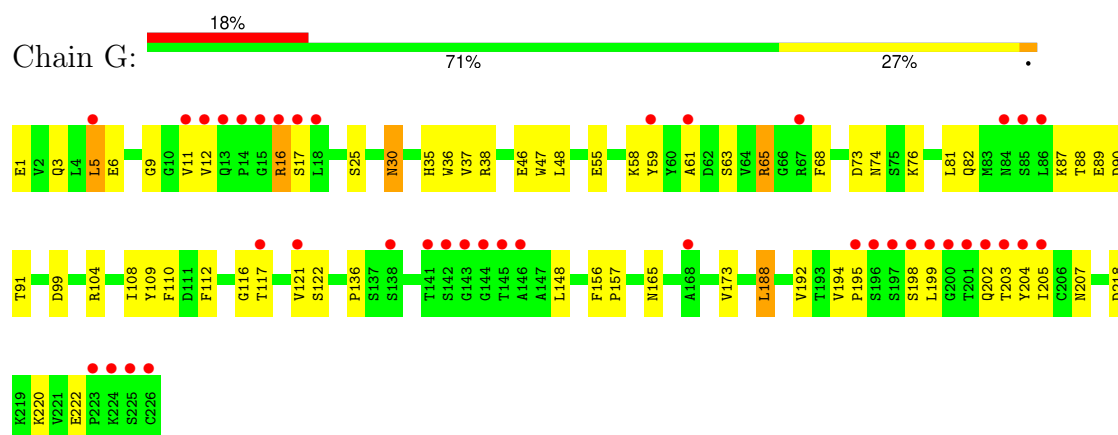
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



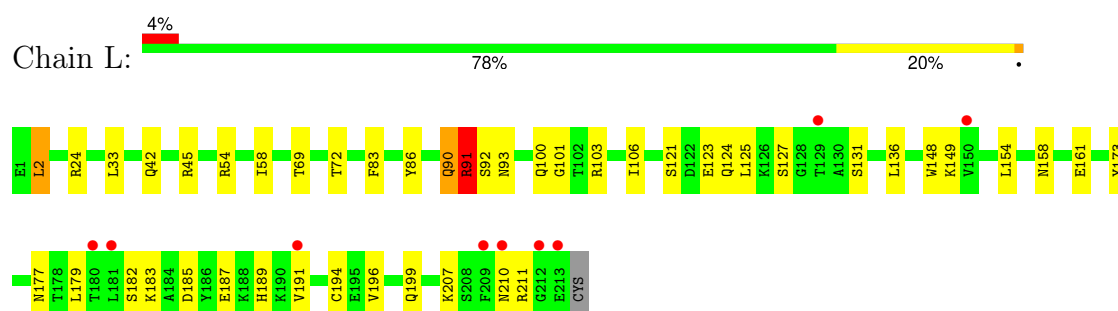
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



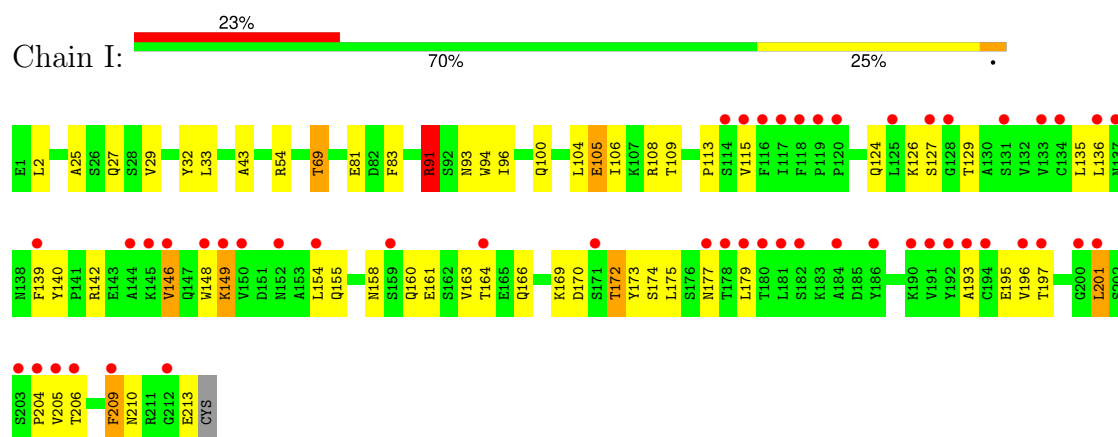
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



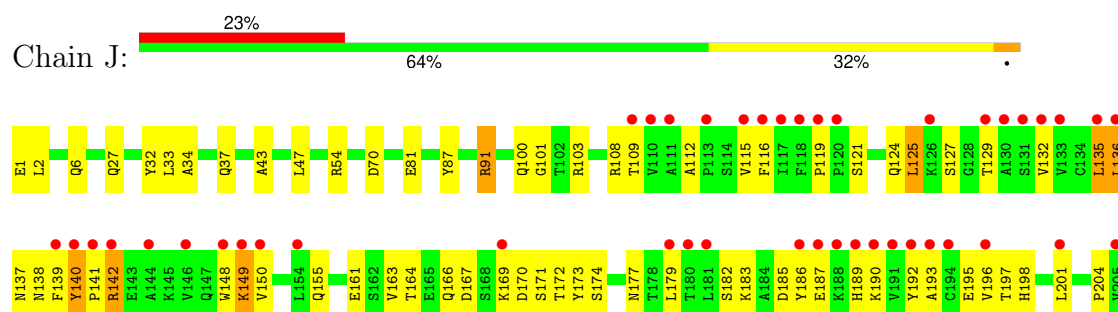
• Molecule 2: HCV1-C1 Antibody Fab Light Chain



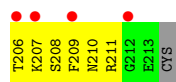
• Molecule 2: HCV1-C1 Antibody Fab Light Chain



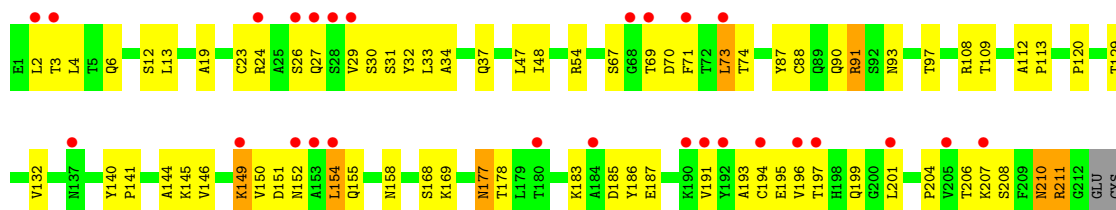
• Molecule 2: HCV1-C1 Antibody Fab Light Chain



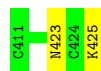
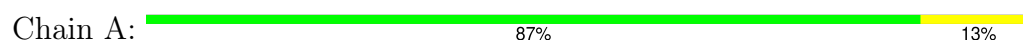




• Molecule 2: HCV1-C1 Antibody Fab Light Chain



• Molecule 3: C1 Epitope



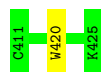
• Molecule 3: C1 Epitope



• Molecule 3: C1 Epitope



• Molecule 3: C1 Epitope



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.07Å 94.54Å 126.76Å 91.84° 94.95° 97.91°	Depositor
Resolution (Å)	29.49 – 2.26 29.49 – 2.26	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.49-2.26) 85.3 (29.49-2.26)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.10pre_2124	Depositor
R, $R_{free}$	0.218 , 0.261 0.219 , 0.261	Depositor DCC
$R_{free}$ test set	4685 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 70.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.73% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CA

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	E	0.80	4/1774 (0.2%)	1.12	20/2416 (0.8%)
1	F	0.56	1/1780 (0.1%)	0.94	4/2422 (0.2%)
1	G	0.52	0/1779	0.84	5/2421 (0.2%)
1	H	0.61	3/1792 (0.2%)	0.75	1/2438 (0.0%)
2	I	0.64	5/1708 (0.3%)	0.85	6/2320 (0.3%)
2	J	0.60	0/1707	0.78	3/2319 (0.1%)
2	K	0.57	2/1663 (0.1%)	1.06	4/2263 (0.2%)
2	L	0.59	0/1702	0.79	3/2312 (0.1%)
3	A	0.55	0/122	0.66	0/163
3	B	0.62	0/130	0.66	0/174
3	C	0.46	0/130	0.64	0/174
3	D	0.57	0/122	0.58	0/163
All	All	0.61	15/14409 (0.1%)	0.89	46/19585 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
2	J	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	6	GLU	CD-OE2	-19.62	1.04	1.25
1	E	6	GLU	CD-OE1	-12.29	1.12	1.25
1	F	96	CYS	CB-SG	-6.84	1.70	1.82
2	I	209	PHE	CB-CG	-6.56	1.40	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	96	CYS	CB-SG	-6.23	1.71	1.82
1	E	216	LYS	CD-CE	5.98	1.66	1.51
2	I	209	PHE	CG-CD2	-5.74	1.30	1.38
2	I	105	GLU	CD-OE1	-5.62	1.19	1.25
2	I	209	PHE	CD2-CE2	-5.48	1.28	1.39
1	E	194	VAL	C-O	5.47	1.33	1.23
2	K	194	CYS	CB-SG	-5.36	1.73	1.81
1	H	140	SER	CB-OG	-5.33	1.35	1.42
1	H	222	GLU	C-O	5.17	1.33	1.23
2	I	195	GLU	CD-OE2	-5.11	1.20	1.25
2	K	149	LYS	CE-NZ	5.06	1.61	1.49

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	73	LEU	CB-CG-CD2	-24.22	69.82	111.00
2	K	73	LEU	CB-CG-CD1	23.20	150.45	111.00
1	F	185	LEU	CB-CG-CD1	-18.74	79.15	111.00
1	F	185	LEU	CB-CG-CD2	18.34	142.18	111.00
1	E	185	LEU	CB-CG-CD2	-13.99	87.22	111.00
1	E	87	LYS	CB-CG-CD	10.94	140.03	111.60
1	E	151	LEU	CA-CB-CG	10.49	139.42	115.30
2	L	2	LEU	CB-CG-CD1	-10.09	93.85	111.00
2	I	201	LEU	CB-CG-CD2	-10.08	93.86	111.00
1	F	185	LEU	CD1-CG-CD2	-9.69	81.42	110.50
2	I	146	VAL	CG1-CB-CG2	9.42	125.97	110.90
1	E	67	ARG	CB-CG-CD	-9.15	87.80	111.60
1	E	67	ARG	NE-CZ-NH1	-9.15	115.72	120.30
1	G	5	LEU	CA-CB-CG	8.88	135.74	115.30
1	E	12	VAL	CG1-CB-CG2	8.81	125.00	110.90
1	E	151	LEU	CB-CG-CD1	-8.69	96.22	111.00
2	L	91	ARG	NE-CZ-NH1	-8.17	116.22	120.30
1	E	216	LYS	CD-CE-NZ	-7.72	93.94	111.70
1	E	199	LEU	CB-CG-CD2	-7.63	98.03	111.00
2	K	73	LEU	CD1-CG-CD2	-7.51	87.97	110.50
2	K	73	LEU	CA-CB-CG	-7.40	98.28	115.30
1	E	115	LEU	CB-CG-CD1	-7.36	98.49	111.00
1	E	67	ARG	CG-CD-NE	6.88	126.25	111.80
2	I	195	GLU	CA-CB-CG	6.76	128.27	113.40
1	E	119	VAL	CG1-CB-CG2	-6.54	100.44	110.90
2	J	142	ARG	NE-CZ-NH2	6.50	123.55	120.30
2	L	91	ARG	NE-CZ-NH2	6.41	123.50	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	ARG	CD-NE-CZ	6.23	132.33	123.60
1	E	83	MET	CA-CB-CG	6.17	123.80	113.30
1	E	199	LEU	CB-CG-CD1	6.06	121.30	111.00
2	I	172	THR	CA-CB-CG2	5.84	120.58	112.40
1	E	173	VAL	CG1-CB-CG2	-5.79	101.64	110.90
1	G	199	LEU	CB-CG-CD2	-5.56	101.56	111.00
1	E	64	VAL	CG1-CB-CG2	-5.45	102.17	110.90
2	J	135	LEU	CA-CB-CG	5.45	127.84	115.30
1	G	188	LEU	CA-CB-CG	5.42	127.77	115.30
1	F	185	LEU	CA-CB-CG	5.37	127.65	115.30
2	J	136	LEU	CA-CB-CG	5.36	127.62	115.30
2	I	91	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	G	65	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	H	73	ASP	CB-CG-OD2	5.20	122.98	118.30
2	I	172	THR	OG1-CB-CG2	5.15	121.85	110.00
1	E	66	GLY	C-N-CA	-5.10	108.96	121.70
1	G	16	ARG	CA-CB-CG	5.08	124.59	113.40
1	E	67	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	E	194	VAL	C-N-CD	-5.01	109.59	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	67	ARG	Sidechain
2	J	125	LEU	Peptide

## 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	E	1727	0	1681	93	0
1	F	1734	0	1705	48	0
1	G	1733	0	1696	74	0
1	H	1742	0	1709	26	0
2	I	1661	0	1626	64	0
2	J	1660	0	1617	80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1625	0	1567	73	0
2	L	1658	0	1616	36	0
3	A	120	0	111	1	0
3	B	125	0	117	1	0
3	C	125	0	117	1	0
3	D	120	0	111	3	0
4	E	4	0	3	7	0
4	F	4	0	3	2	0
4	G	4	0	3	2	0
4	H	4	0	3	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	4	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
5	I	1	0	0	0	0
5	J	2	0	0	0	0
5	K	5	0	0	0	0
5	L	2	0	0	0	0
6	A	7	0	0	0	0
6	B	10	0	0	1	0
6	C	6	0	0	1	0
6	D	3	0	0	0	0
6	E	48	0	0	12	0
6	F	68	0	0	8	0
6	G	60	0	0	18	0
6	H	83	0	0	3	0
6	I	53	0	0	6	0
6	J	76	0	0	7	0
6	K	49	0	0	15	0
6	L	85	0	0	8	0
All	All	14615	0	13685	481	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 17.

All (481) 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:170:ASP:OD2	2:I:172:THR:HG23	1.09	1.25

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:VAL:HG12	6:E:406:HOH:O	1.18	1.25
2:L:2:LEU:HD11	2:L:93:ASN:HB3	1.31	1.10
2:I:170:ASP:OD2	2:I:172:THR:CG2	1.99	1.08
1:F:205:ILE:HD12	1:F:220:LYS:HD2	1.33	1.07
2:K:195:GLU:HG3	2:K:206:THR:HG23	1.35	1.03
1:E:68:PHE:CD2	1:E:83:MET:HB2	1.93	1.02
2:J:195:GLU:OE1	2:J:206:THR:OG1	1.78	0.99
1:E:126:THR:O	1:E:127:LYS:HE2	1.61	0.99
1:F:205:ILE:HD11	1:F:218:ASP:HB3	1.41	0.98
1:E:145:THR:HA	1:E:195:PRO:HA	1.45	0.97
1:H:3:GLN:NE2	6:H:401:HOH:O	1.98	0.95
1:G:16:ARG:HD3	1:G:17:SER:H	1.27	0.95
2:K:191:VAL:O	6:K:401:HOH:O	1.85	0.95
2:I:155:GLN:HB3	2:I:158:ASN:HD21	1.32	0.95
2:K:191:VAL:HG12	2:K:210:ASN:HD22	1.32	0.94
2:J:149:LYS:HD3	2:J:193:ALA:HB3	1.50	0.94
1:G:46:GLU:OE2	6:G:401:HOH:O	1.86	0.94
2:K:186:TYR:O	2:K:211:ARG:NH2	2.01	0.94
2:K:145:LYS:HB3	2:K:197:THR:HG22	1.50	0.93
2:J:150:VAL:HG23	2:J:155:GLN:NE2	1.84	0.92
2:K:195:GLU:HG3	2:K:206:THR:CG2	2.00	0.91
2:I:149:LYS:HE3	2:I:193:ALA:HB3	1.53	0.90
2:I:169:LYS:NZ	6:I:401:HOH:O	2.04	0.89
2:L:2:LEU:HB3	6:L:468:HOH:O	1.75	0.87
1:G:16:ARG:CD	1:G:17:SER:H	1.87	0.87
1:G:36:TRP:O	6:G:402:HOH:O	1.93	0.86
1:E:180:LEU:O	2:I:160:GLN:NE2	2.07	0.86
2:K:195:GLU:CG	2:K:206:THR:HG23	2.04	0.85
1:G:198:SER:OG	6:G:403:HOH:O	1.94	0.85
2:K:24:ARG:NH2	2:K:70:ASP:OD1	2.09	0.85
1:G:90:ASP:OD1	6:G:404:HOH:O	1.95	0.85
1:E:165:ASN:HD21	1:E:169:LEU:HB3	1.40	0.85
2:L:2:LEU:CD1	2:L:93:ASN:HB3	2.07	0.84
2:J:150:VAL:CG2	2:J:155:GLN:NE2	2.40	0.84
1:E:64:VAL:HG13	1:E:68:PHE:CD1	2.13	0.84
3:C:411:CYS:N	6:C:601:HOH:O	2.10	0.84
1:E:6:GLU:OE1	1:E:114:GLY:HA3	1.78	0.84
2:K:32:TYR:HB3	2:K:91:ARG:HG3	1.60	0.84
1:F:205:ILE:HD12	1:F:220:LYS:CD	2.08	0.83
1:E:136:PRO:HB2	1:E:199:LEU:HD21	1.61	0.83
2:K:97:THR:O	6:K:403:HOH:O	1.96	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:142:ARG:HH21	2:J:163:VAL:HB	1.42	0.82
2:L:148:TRP:NE1	2:L:177:ASN:OD1	2.14	0.80
2:J:140:TYR:CD2	2:J:141:PRO:HA	2.16	0.80
1:E:205:ILE:HD11	1:E:218:ASP:HB3	1.63	0.80
2:J:148:TRP:NE1	2:J:177:ASN:OD1	2.14	0.80
2:K:6:GLN:HE22	2:K:87:TYR:HA	1.46	0.80
2:I:164:THR:HG22	2:I:174:SER:H	1.45	0.79
1:E:63:SER:O	1:E:64:VAL:HG23	1.82	0.79
2:J:150:VAL:HG23	2:J:155:GLN:HE21	1.46	0.78
2:K:129:THR:OG1	6:K:404:HOH:O	2.02	0.78
1:G:88:THR:HA	1:G:121:VAL:HG13	1.65	0.78
1:E:154:ASP:OD1	1:E:185:LEU:HD21	1.84	0.77
3:B:411:CYS:N	6:B:501:HOH:O	2.16	0.77
1:E:13:GLN:N	6:E:406:HOH:O	2.17	0.77
1:E:64:VAL:CG1	1:E:68:PHE:CD1	2.67	0.76
2:K:191:VAL:HG12	2:K:210:ASN:ND2	2.01	0.76
1:G:3:GLN:O	6:G:405:HOH:O	2.04	0.76
2:K:168:SER:OG	6:K:405:HOH:O	2.04	0.75
1:H:1:GLU:N	6:H:402:HOH:O	2.19	0.75
2:I:108:ARG:NH1	2:I:109:THR:OG1	2.12	0.75
1:E:131:VAL:HG21	1:E:217:VAL:HG21	1.67	0.74
2:K:199:GLN:OE1	6:K:406:HOH:O	2.05	0.74
1:F:205:ILE:CD1	1:F:220:LYS:HD2	2.14	0.74
1:E:165:ASN:ND2	1:E:169:LEU:HB3	2.02	0.73
1:G:63:SER:O	6:G:406:HOH:O	2.05	0.73
2:I:106:ILE:H	2:I:166:GLN:HE22	1.34	0.73
2:L:161:GLU:HB3	2:L:177:ASN:HD22	1.54	0.72
2:I:2[B]:LEU:HD21	2:I:29:VAL:HG12	1.70	0.72
2:I:209:PHE:HZ	2:I:213:GLU:HB3	1.53	0.72
1:E:12:VAL:HG21	1:E:18:LEU:CD1	2.19	0.72
1:E:40:THR:HG23	1:E:43:LYS:H	1.55	0.72
2:J:140:TYR:HD2	2:J:141:PRO:CA	2.01	0.72
2:K:29:VAL:HG11	2:K:90:GLN:HG3	1.71	0.72
1:F:1:GLU:OE1	1:F:1:GLU:N	2.16	0.72
1:E:83:MET:HG3	1:E:86:LEU:HD21	1.72	0.71
1:G:194:VAL:HG12	1:G:195:PRO:HD2	1.72	0.71
2:K:90:GLN:NE2	2:K:93:ASN:H	1.87	0.71
1:G:16:ARG:HD3	1:G:17:SER:N	2.04	0.71
1:E:165:ASN:OD1	1:E:169:LEU:N	2.24	0.71
1:E:87:LYS:HG3	1:E:88:THR:H	1.54	0.70
1:G:16:ARG:NH2	6:G:408:HOH:O	2.19	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:GLY:O	6:E:402:HOH:O	2.08	0.70
1:F:156:PHE:HB2	1:F:185:LEU:HD11	1.73	0.70
2:J:108:ARG:HG3	2:J:140:TYR:CD1	2.25	0.70
1:E:91:THR:HG22	6:E:401:HOH:O	1.91	0.70
1:F:205:ILE:CD1	1:F:218:ASP:HB3	2.20	0.70
2:J:125:LEU:HD23	2:J:183:LYS:HG3	1.74	0.69
1:H:194:VAL:HG11	1:H:204:TYR:OH	1.92	0.69
2:K:149:LYS:NZ	2:K:193:ALA:HB3	2.07	0.69
1:F:213:SER:O	6:F:401:HOH:O	2.08	0.69
2:J:70[B]:ASP:OD1	6:J:401:HOH:O	2.10	0.69
1:E:68:PHE:CG	1:E:83:MET:HB2	2.28	0.68
2:L:207:LYS:HE3	2:L:207:LYS:HA	1.75	0.68
1:E:224:LYS:NZ	6:E:404:HOH:O	2.14	0.68
1:F:205:ILE:HD11	1:F:218:ASP:CB	2.22	0.68
1:H:43:LYS:HA	1:H:43:LYS:HE2	1.76	0.68
2:L:207:LYS:O	6:L:401:HOH:O	2.11	0.67
1:G:63:SER:N	6:G:410:HOH:O	2.26	0.67
1:G:35:HIS:HD2	1:G:47:TRP:HE1	1.43	0.67
2:K:183:LYS:HA	2:K:186:TYR:HB3	1.76	0.67
2:I:149:LYS:CE	2:I:193:ALA:HB3	2.24	0.67
1:G:91:THR:O	6:G:407:HOH:O	2.12	0.67
1:G:9:GLY:H	1:G:117:THR:HG21	1.59	0.67
2:K:90:GLN:HE21	2:K:93:ASN:H	1.41	0.67
2:J:140:TYR:HD2	2:J:141:PRO:N	1.93	0.67
2:K:145:LYS:HB3	2:K:197:THR:CG2	2.25	0.67
2:K:150:VAL:HA	6:K:401:HOH:O	1.94	0.67
2:J:139:PHE:CE2	2:J:142:ARG:HA	2.30	0.66
2:K:149:LYS:HZ3	2:K:193:ALA:HB3	1.61	0.66
1:E:86:LEU:HB3	1:E:121:VAL:HG21	1.78	0.66
2:I:209:PHE:CZ	2:I:213:GLU:HB3	2.30	0.66
2:K:91:ARG:NH1	6:K:402:HOH:O	1.91	0.66
1:H:133:PRO:HB3	1:H:221:VAL:HG12	1.78	0.66
2:K:144:ALA:O	6:K:407:HOH:O	2.14	0.65
1:F:104:ARG:H	4:F:301:ACT:H1	1.59	0.65
1:F:133:PRO:HB3	1:F:219:LYS:HZ3	1.62	0.65
1:F:169:LEU:HD21	1:F:192:VAL:HG21	1.79	0.65
2:I:43:ALA:O	6:I:403:HOH:O	2.14	0.64
1:E:19:ARG:NH1	6:E:409:HOH:O	2.30	0.64
1:E:213:SER:O	1:E:215:THR:N	2.31	0.64
2:I:2[A]:LEU:CD1	2:I:93:ASN:HB3	2.27	0.64
2:J:6:GLN:HE22	2:J:87:TYR:HA	1.63	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:LYS:NZ	1:G:89:GLU:OE1	2.24	0.63
1:G:104[A]:ARG:NH2	6:G:411:HOH:O	2.26	0.63
2:J:142:ARG:HH21	2:J:163:VAL:CB	2.09	0.63
2:K:27:GLN:O	6:K:408:HOH:O	2.15	0.63
2:K:108:ARG:NH1	2:K:109:THR:OG1	2.31	0.63
2:L:194:CYS:N	6:L:401:HOH:O	2.31	0.62
1:E:213:SER:O	1:E:213:SER:OG	2.16	0.62
2:J:149:LYS:H	2:J:149:LYS:HD2	1.64	0.62
2:I:161:GLU:HB3	2:I:177:ASN:HD22	1.65	0.62
2:J:108:ARG:NH1	2:J:109:THR:OG1	2.33	0.62
1:H:104:ARG:HE	4:E:301:ACT:H1	1.65	0.61
1:E:88:THR:O	1:E:91:THR:HG23	2.00	0.61
2:J:132:VAL:CG1	2:J:179:LEU:HB3	2.29	0.61
2:K:90:GLN:HB2	6:K:436:HOH:O	1.99	0.61
1:G:37:VAL:HG22	6:G:402:HOH:O	1.99	0.61
2:I:155:GLN:OE1	2:I:158:ASN:ND2	2.34	0.61
2:J:142:ARG:NH2	2:J:163:VAL:HB	2.13	0.61
2:K:195:GLU:CD	2:K:206:THR:HG23	2.20	0.61
2:I:136:LEU:HD13	2:I:175:LEU:HD22	1.81	0.61
2:J:140:TYR:CD2	2:J:141:PRO:CA	2.79	0.61
2:L:189:HIS:O	2:L:211:ARG:NH2	2.19	0.61
1:G:104[B]:ARG:H	4:G:301:ACT:H2	1.64	0.61
2:L:2:LEU:HD11	2:L:93:ASN:CB	2.21	0.61
2:J:163:VAL:HG13	2:J:174:SER:O	2.00	0.61
1:E:62:ASP:OD1	1:E:65:ARG:NH1	2.34	0.61
1:G:194:VAL:CG1	1:G:195:PRO:HD2	2.30	0.61
1:E:129:PRO:HB3	1:E:155:TYR:HB3	1.83	0.60
1:G:104[A]:ARG:H	4:G:301:ACT:H2	1.64	0.60
1:F:104:ARG:HG3	4:F:301:ACT:H3	1.82	0.60
1:G:87:LYS:HZ1	1:G:89:GLU:CD	2.05	0.60
1:F:174:HIS:HE1	2:J:138:ASN:OD1	1.83	0.60
2:I:2[B]:LEU:HD21	2:I:29:VAL:CG1	2.31	0.60
2:K:69:THR:HG22	6:K:408:HOH:O	2.01	0.60
2:K:4:LEU:HD12	6:K:403:HOH:O	2.02	0.59
1:G:202:GLN:OE1	1:G:203:THR:N	2.27	0.59
2:K:37:GLN:HB2	2:K:47:LEU:HD11	1.82	0.59
1:E:94:TYR:CD1	1:E:119:VAL:CG2	2.85	0.59
2:L:191:VAL:CG1	2:L:210:ASN:OD1	2.50	0.59
1:G:38:ARG:HD3	1:G:48:LEU:HD21	1.83	0.59
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.85	0.58
1:G:87:LYS:HD2	1:G:88:THR:N	2.19	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:SER:O	1:H:199:LEU:HD13	2.02	0.58
1:E:87:LYS:CG	1:E:88:THR:N	2.65	0.58
1:E:12:VAL:CG2	1:E:18:LEU:CD1	2.82	0.58
1:E:64:VAL:HG11	1:E:68:PHE:CD1	2.39	0.58
2:I:2[A]:LEU:HD11	2:I:93:ASN:HB3	1.84	0.58
2:J:132:VAL:HG12	2:J:179:LEU:HB3	1.86	0.58
1:E:87:LYS:HG3	1:E:88:THR:N	2.19	0.58
1:F:156:PHE:HB2	1:F:185:LEU:CD1	2.33	0.58
1:F:191:VAL:HG11	2:J:135:LEU:HD12	1.85	0.58
1:G:194:VAL:HG11	1:G:204:TYR:OH	2.04	0.58
2:J:149:LYS:HD2	2:J:149:LYS:N	2.19	0.57
2:I:105:GLU:HG2	2:I:106:ILE:N	2.19	0.57
2:J:1:GLU:O	6:J:402:HOH:O	2.17	0.57
1:G:205:ILE:HD11	1:G:218:ASP:C	2.25	0.57
2:J:170:ASP:OD1	2:J:172:THR:HG22	2.04	0.57
1:G:12:VAL:O	1:G:121:VAL:HA	2.05	0.57
1:E:93:MET:HG2	6:E:403:HOH:O	2.04	0.56
2:I:100:GLN:O	6:I:404:HOH:O	2.17	0.56
1:G:112:PHE:HB3	6:G:435:HOH:O	2.03	0.56
2:K:120:PRO:HD3	2:K:132:VAL:HG22	1.87	0.56
2:I:155:GLN:HB3	2:I:158:ASN:ND2	2.14	0.56
1:H:108:ILE:HB	2:L:91:ARG:HD2	1.87	0.56
2:I:161:GLU:HB3	2:I:177:ASN:ND2	2.20	0.56
2:J:142:ARG:HD2	2:J:173:TYR:CE1	2.41	0.56
1:G:87:LYS:NZ	1:G:88:THR:HG22	2.20	0.56
1:F:43:LYS:NZ	6:F:406:HOH:O	2.35	0.56
2:K:177:ASN:HD22	2:K:178:THR:N	2.03	0.56
2:I:158:ASN:OD1	2:I:158:ASN:N	2.38	0.56
1:E:188:LEU:HD12	1:E:189:SER:N	2.21	0.56
1:G:198:SER:HB2	6:G:422:HOH:O	2.06	0.56
2:L:103:ARG:NH1	2:L:173:TYR:OH	2.36	0.55
1:E:132:PHE:CD1	2:I:124:GLN:HB2	2.41	0.55
2:I:113:PRO:HD2	2:I:201:LEU:CD1	2.35	0.55
2:J:150:VAL:HG21	2:J:155:GLN:NE2	2.20	0.55
2:L:199:GLN:HB2	6:L:466:HOH:O	2.06	0.55
1:E:103:VAL:H	4:E:301:ACT:CH3	2.19	0.55
2:I:172:THR:HG1	2:I:173:TYR:H	1.53	0.55
1:E:156:PHE:CD1	1:E:157:PRO:HA	2.43	0.54
2:L:123:GLU:OE1	2:L:123:GLU:N	2.31	0.54
1:E:85:SER:O	1:E:85:SER:OG	2.23	0.54
1:E:155:TYR:N	1:E:185:LEU:HD11	2.23	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:183:LYS:HA	2:K:186:TYR:CB	2.37	0.54
1:E:12:VAL:O	1:E:121:VAL:HA	2.08	0.54
1:E:12:VAL:HG21	1:E:18:LEU:HD12	1.89	0.54
2:K:195:GLU:OE2	2:K:204:PRO:HB2	2.08	0.54
2:I:209:PHE:HZ	2:I:213:GLU:CB	2.18	0.54
1:F:170:THR:O	1:F:173:VAL:HG22	2.08	0.54
4:H:301:ACT:H2	4:E:301:ACT:OXT	2.08	0.54
1:E:87:LYS:CG	1:E:88:THR:H	2.21	0.54
2:L:90:GLN:OE1	2:L:92:SER:N	2.42	0.53
2:J:124:GLN:O	2:J:127:SER:N	2.36	0.53
1:F:129:PRO:HB3	1:F:155:TYR:HB3	1.91	0.53
1:G:35:HIS:HD2	1:G:47:TRP:NE1	2.05	0.53
1:G:194:VAL:HG12	6:G:422:HOH:O	2.07	0.53
2:K:3:THR:OG1	2:K:26:SER:HB3	2.08	0.53
2:I:113:PRO:HD2	2:I:201:LEU:HD12	1.91	0.53
2:K:73:LEU:HG	2:K:74:THR:N	2.23	0.53
2:I:164:THR:CG2	2:I:174:SER:H	2.20	0.53
2:J:139:PHE:HE2	2:J:142:ARG:HA	1.73	0.53
2:K:177:ASN:HD22	2:K:178:THR:H	1.53	0.53
1:E:95:TYR:OH	6:E:403:HOH:O	2.12	0.52
2:L:45[A]:ARG:NH1	6:L:403:HOH:O	2.41	0.52
1:G:87:LYS:HZ2	1:G:88:THR:HG22	1.75	0.52
1:E:121:VAL:N	6:E:401:HOH:O	2.00	0.52
2:I:196:VAL:HG12	2:I:205:VAL:O	2.09	0.52
1:E:179:VAL:O	1:E:186:TYR:HA	2.10	0.52
1:E:210:HIS:HD2	1:E:212:PRO:HD2	1.74	0.52
2:I:139:PHE:O	2:I:172:THR:OG1	2.18	0.52
2:J:142:ARG:HH21	2:J:163:VAL:CG1	2.22	0.52
2:J:115:VAL:O	2:J:207:LYS:HG3	2.10	0.51
1:H:170:THR:O	1:H:173:VAL:HG22	2.09	0.51
1:E:134:LEU:HD21	1:E:151:LEU:HD22	1.91	0.51
1:H:11:VAL:HG21	1:H:157:PRO:HG3	1.93	0.51
1:F:133:PRO:HB3	1:F:219:LYS:NZ	2.26	0.51
1:F:205:ILE:CD1	1:F:220:LYS:CD	2.83	0.51
2:J:161:GLU:HB3	2:J:177:ASN:HD22	1.74	0.51
1:G:58:LYS:O	1:G:59:TYR:HD1	1.92	0.51
1:E:94:TYR:CE1	1:E:119:VAL:HG23	2.46	0.51
1:F:139:LYS:NZ	6:F:404:HOH:O	2.32	0.51
2:J:108:ARG:HG3	2:J:140:TYR:CE1	2.44	0.51
1:G:1:GLU:OE2	1:G:3:GLN:NE2	2.44	0.51
2:L:124:GLN:O	2:L:127:SER:OG	2.20	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:PHE:CE2	1:E:83:MET:HB2	2.42	0.51
1:G:38:ARG:HB3	1:G:48:LEU:HD11	1.93	0.51
2:J:167[A]:ASP:OD2	2:J:169:LYS:HB2	2.10	0.51
2:L:131:SER:HA	2:L:179:LEU:O	2.11	0.51
1:F:83:MET:HB3	1:F:86:LEU:HD21	1.91	0.51
1:F:220:LYS:HD3	1:F:220:LYS:N	2.26	0.51
1:G:35:HIS:HE1	1:G:99:ASP:HB2	1.75	0.51
1:H:38:ARG:HD3	1:H:48:LEU:HD11	1.93	0.51
2:K:48:ILE:HD13	2:K:54:ARG:HA	1.93	0.51
1:E:94:TYR:CE1	1:E:119:VAL:CG2	2.93	0.50
2:I:108:ARG:NE	2:I:109:THR:O	2.41	0.50
1:G:87:LYS:HE3	1:G:89:GLU:HB2	1.92	0.50
2:L:149:LYS:HG2	2:L:154:LEU:HD23	1.92	0.50
1:F:219:LYS:NZ	1:F:221:VAL:HG22	2.26	0.50
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.91	0.50
1:G:25:SER:N	6:G:405:HOH:O	2.29	0.50
2:K:33:LEU:HD23	2:K:34:ALA:N	2.27	0.50
2:L:183:LYS:HE2	2:L:187:GLU:OE2	2.12	0.50
2:J:124:GLN:O	2:J:127:SER:HB2	2.12	0.50
2:K:4:LEU:HD13	2:K:88:CYS:SG	2.51	0.50
1:F:83:MET:HE2	1:F:86:LEU:HD21	1.94	0.50
2:J:189:HIS:O	2:J:211:ARG:NH1	2.44	0.50
2:K:113:PRO:HD2	2:K:201:LEU:CD1	2.41	0.50
2:I:105:GLU:OE2	2:I:140:TYR:OH	2.27	0.50
2:J:100:GLN:HG2	6:J:423:HOH:O	2.11	0.50
2:J:172:THR:HG23	6:J:413:HOH:O	2.11	0.50
2:I:115:VAL:HA	2:I:135:LEU:O	2.11	0.50
1:F:147:ALA:HB3	2:J:116:PHE:HD2	1.78	0.49
1:F:205:ILE:HA	1:F:220:LYS:HA	1.94	0.49
1:G:173:VAL:HG22	1:G:192:VAL:CG1	2.42	0.49
2:L:42:GLN:OE1	6:L:402:HOH:O	2.20	0.49
2:L:182:SER:OG	2:L:185:ASP:OD1	2.29	0.49
2:J:2:LEU:HD23	2:J:2:LEU:N	2.26	0.49
1:G:108:ILE:HB	2:K:91:ARG:HD2	1.95	0.49
1:E:180:LEU:HD12	1:E:181:GLN:O	2.13	0.49
1:G:220:LYS:NZ	1:G:222:GLU:OE2	2.33	0.49
1:H:105:ASP:HB3	6:H:467:HOH:O	2.13	0.49
2:K:33:LEU:HD13	2:K:71:PHE:CG	2.48	0.49
1:E:162:VAL:HG22	1:E:208:VAL:HG22	1.94	0.49
2:J:119:PRO:HG3	2:J:209:PHE:CG	2.48	0.49
1:E:62:ASP:O	1:E:63:SER:OG	2.23	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:LYS:HZ2	1:F:221:VAL:HG22	1.77	0.49
2:J:182:SER:OG	2:J:185:ASP:OD2	2.18	0.49
2:K:4:LEU:HD13	2:K:23:CYS:SG	2.53	0.48
1:E:68:PHE:HA	6:E:411:HOH:O	2.12	0.48
2:J:6:GLN:NE2	2:J:101:GLY:H	2.10	0.48
1:E:6:GLU:HA	1:E:21:SER:O	2.14	0.48
1:E:46:GLU:OE1	6:E:407:HOH:O	2.20	0.48
1:E:103:VAL:H	4:E:301:ACT:H2	1.78	0.48
1:G:59:TYR:HD2	3:D:420:TRP:HZ3	1.59	0.48
2:L:121:SER:HB2	2:L:123:GLU:OE1	2.14	0.48
1:E:55:GLU:OE2	1:E:72:ARG:O	2.32	0.48
1:E:208:VAL:HB	1:E:217:VAL:HG22	1.96	0.48
1:F:151:LEU:HD13	6:F:402:HOH:O	2.13	0.48
2:K:4:LEU:HD11	6:K:436:HOH:O	2.12	0.48
1:E:12:VAL:CG2	1:E:18:LEU:HD11	2.43	0.48
2:K:149:LYS:CD	2:K:193:ALA:HB3	2.43	0.48
2:K:193:ALA:HB2	2:K:208:SER:HB3	1.95	0.48
1:E:12:VAL:HG21	1:E:18:LEU:CG	2.44	0.48
1:G:87:LYS:HZ2	1:G:89:GLU:H	1.61	0.48
1:G:61:ALA:HA	6:G:415:HOH:O	2.13	0.48
1:G:47:TRP:HA	6:G:402:HOH:O	2.13	0.47
1:F:133:PRO:HD2	2:J:121:SER:CB	2.44	0.47
2:J:2:LEU:HD22	2:J:27:GLN:HG2	1.95	0.47
1:H:133:PRO:HD2	2:L:121:SER:CB	2.44	0.47
1:F:8:GLY:O	1:F:18[B]:LEU:HD11	2.14	0.47
1:H:12:VAL:HG11	1:H:18:LEU:HG	1.96	0.47
3:A:423:ASN:OD1	3:A:425:LYS:NZ	2.47	0.47
2:I:155:GLN:CB	2:I:158:ASN:HD21	2.17	0.47
1:G:109:TYR:CD1	2:K:34:ALA:HB2	2.50	0.47
2:I:148:TRP:NE1	2:I:177:ASN:OD1	2.35	0.47
1:G:30:ASN:ND2	1:G:74:ASN:HB3	2.29	0.47
2:I:146:VAL:HG21	2:I:177:ASN:ND2	2.30	0.47
2:I:193:ALA:HB1	2:I:206:THR:CG2	2.44	0.47
2:J:103[B]:ARG:HH12	2:J:166:GLN:HB2	1.79	0.47
1:G:194:VAL:HG12	1:G:195:PRO:CD	2.43	0.47
1:G:68:PHE:HA	1:G:82:GLN:O	2.14	0.47
1:E:136:PRO:HG3	1:E:148:LEU:HB3	1.97	0.47
2:K:149:LYS:CG	2:K:193:ALA:HB3	2.44	0.47
2:K:183:LYS:O	2:K:187:GLU:HG2	2.14	0.47
2:J:169:LYS:NZ	6:J:409:HOH:O	2.42	0.46
2:K:207:LYS:HD3	2:K:208:SER:H	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:VAL:HG11	1:F:204:TYR:CZ	2.49	0.46
2:J:108:ARG:CG	2:J:140:TYR:CD1	2.96	0.46
2:K:169:LYS:HG2	6:K:405:HOH:O	2.14	0.46
1:E:199:LEU:HG	1:E:223:PRO:HG3	1.98	0.46
1:H:204:TYR:O	1:H:205:ILE:HD13	2.15	0.46
1:E:36:TRP:CZ2	1:E:79:LEU:HD23	2.50	0.46
1:E:12:VAL:HG21	1:E:18:LEU:HG	1.98	0.46
1:F:115:LEU:HD12	1:F:115:LEU:H	1.81	0.46
1:E:64:VAL:HG11	1:E:68:PHE:HD1	1.79	0.46
2:I:25:ALA:O	2:I:69:THR:OG1	2.33	0.46
2:L:54:ARG:HD2	2:L:58:ILE:O	2.16	0.46
2:I:2[A]:LEU:CD2	2:I:27:GLN:HG2	2.45	0.46
1:G:173:VAL:HG22	1:G:192:VAL:HG12	1.98	0.46
1:E:154:ASP:HA	1:E:185:LEU:HD11	1.98	0.46
1:F:219:LYS:HE3	1:F:219:LYS:HB3	1.75	0.46
2:J:135:LEU:CD2	2:J:137:ASN:HB2	2.45	0.46
2:K:154:LEU:HD12	2:K:154:LEU:H	1.80	0.45
2:I:83:PHE:CD1	2:I:104:LEU:HD22	2.51	0.45
2:J:197:THR:HG23	2:J:204:PRO:HG3	1.99	0.45
1:H:126:THR:HA	1:H:156:PHE:O	2.17	0.45
2:I:209:PHE:CD1	2:I:210:ASN:N	2.82	0.45
1:F:109:TYR:CD1	2:J:34:ALA:HB2	2.52	0.45
2:J:81:GLU:CD	2:J:81:GLU:H	2.20	0.45
1:G:87:LYS:HD2	1:G:87:LYS:C	2.37	0.45
1:E:114:GLY:O	2:I:43:ALA:HB2	2.16	0.45
1:E:132:PHE:CE1	2:I:124:GLN:HB2	2.51	0.45
2:J:33:LEU:HG	2:J:34:ALA:N	2.32	0.45
1:F:205:ILE:HG13	1:F:219:LYS:C	2.38	0.45
2:K:149:LYS:HE2	2:K:152:ASN:ND2	2.32	0.45
1:H:68:PHE:HA	1:H:82:GLN:O	2.17	0.45
1:H:104:ARG:HE	4:E:301:ACT:CH3	2.28	0.45
1:E:103:VAL:HG23	4:E:301:ACT:H3	1.99	0.45
2:I:136:LEU:HD22	2:I:175:LEU:HD13	1.98	0.45
2:J:124:GLN:HG2	2:J:129:THR:O	2.16	0.45
2:K:149:LYS:NZ	2:K:193:ALA:CB	2.77	0.45
2:L:191:VAL:HG12	2:L:210:ASN:OD1	2.16	0.44
1:E:188:LEU:HD12	1:E:189:SER:H	1.81	0.44
1:F:108:ILE:HB	2:J:91:ARG:HD2	1.98	0.44
2:K:112:ALA:HB1	2:K:201:LEU:HD11	1.98	0.44
1:E:210:HIS:CD2	1:E:212:PRO:HD2	2.50	0.44
1:F:136:PRO:HD3	1:F:221:VAL:HG12	2.00	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:100:GLN:NE2	6:J:406:HOH:O	2.32	0.44
1:G:65:ARG:HA	6:G:442:HOH:O	2.16	0.44
1:G:165:ASN:OD1	1:G:205:ILE:HG22	2.18	0.44
1:E:13:GLN:O	6:E:406:HOH:O	2.21	0.44
2:J:32:TYR:HB3	2:J:91:ARG:HG3	2.00	0.44
2:J:198:HIS:HB3	2:J:201:LEU:CD2	2.47	0.44
2:K:151:ASP:HA	2:K:191:VAL:HG23	1.99	0.44
1:F:38:ARG:HD3	1:F:48:LEU:HD11	1.99	0.44
2:K:29:VAL:O	2:K:31:SER:N	2.51	0.44
2:L:83:PHE:CZ	2:L:106:ILE:HD13	2.53	0.44
2:I:32:TYR:HB3	2:I:91:ARG:HG3	2.00	0.44
2:J:136:LEU:HD21	2:J:196:VAL:HG21	2.00	0.44
1:E:36:TRP:NE1	1:E:81:LEU:HB2	2.32	0.44
1:G:38:ARG:CD	1:G:48:LEU:HD21	2.47	0.44
1:G:205:ILE:HD11	1:G:218:ASP:HB3	1.99	0.44
2:I:81:GLU:CD	2:I:81:GLU:H	2.21	0.43
2:I:113:PRO:HB3	2:I:139:PHE:HB3	2.00	0.43
1:H:136:PRO:HG3	1:H:148:LEU:HD22	2.00	0.43
2:L:72:THR:HG23	6:L:470:HOH:O	2.18	0.43
1:F:156:PHE:CB	1:F:185:LEU:HD11	2.46	0.43
2:I:124:GLN:HG2	2:I:129:THR:O	2.18	0.43
2:K:4:LEU:HA	2:K:24:ARG:O	2.18	0.43
1:E:210:HIS:CE1	1:E:213:SER:HB3	2.53	0.43
2:I:124:GLN:O	2:I:127:SER:HB2	2.17	0.43
2:I:149:LYS:N	6:I:407:HOH:O	2.40	0.43
1:G:35:HIS:CE1	1:G:99:ASP:HB2	2.53	0.43
1:G:61:ALA:O	1:G:65:ARG:HG2	2.18	0.43
2:K:140:TYR:CD1	2:K:141:PRO:HA	2.53	0.43
2:L:100[A]:GLN:HG2	6:L:442:HOH:O	2.17	0.43
2:I:126:LYS:HD2	2:I:126:LYS:O	2.18	0.43
2:I:172:THR:OG1	2:I:173:TYR:N	2.50	0.43
1:F:174:HIS:CE1	2:J:174:SER:OG	2.72	0.43
1:G:58:LYS:O	1:G:59:TYR:CD1	2.71	0.43
1:F:172:GLY:N	6:F:407:HOH:O	2.35	0.43
1:G:55:GLU:O	1:G:58:LYS:HE2	2.18	0.43
2:I:197:THR:HG23	2:I:204:PRO:HG3	2.01	0.43
2:J:149:LYS:HZ1	2:J:195:GLU:HB2	1.83	0.43
2:L:24:ARG:HA	2:L:69:THR:O	2.18	0.43
1:E:36:TRP:NE1	1:E:79:LEU:HD21	2.33	0.43
1:E:129:PRO:HA	1:E:154:ASP:O	2.19	0.43
2:J:193:ALA:HB1	2:J:206:THR:HG22	2.01	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:SER:N	1:E:153:LYS:O	2.52	0.43
1:G:11:VAL:HG21	1:G:157:PRO:HG3	2.00	0.43
2:J:167[A]:ASP:OD2	2:J:169:LYS:HE2	2.19	0.42
1:G:38:ARG:HE	1:G:46:GLU:HG2	1.83	0.42
1:G:59:TYR:HD2	3:D:420:TRP:CZ3	2.36	0.42
1:H:148:LEU:HD13	1:H:221:VAL:HG21	2.01	0.42
2:I:113:PRO:HD2	2:I:201:LEU:HD11	2.02	0.42
2:L:136:LEU:HD11	2:L:196:VAL:HG11	2.01	0.42
1:H:129:PRO:HB3	1:H:155:TYR:HB3	2.00	0.42
1:E:199:LEU:C	1:E:201:THR:H	2.23	0.42
1:F:1:GLU:N	6:F:413:HOH:O	2.53	0.42
1:H:133:PRO:HD2	2:L:121:SER:HB3	2.01	0.42
2:I:148:TRP:HB3	2:I:179:LEU:HD22	2.01	0.42
2:J:112:ALA:HB2	6:J:443:HOH:O	2.18	0.42
1:H:104:ARG:HH21	4:E:301:ACT:H1	1.85	0.42
2:L:86:TYR:O	2:L:101:GLY:HA2	2.20	0.42
2:I:142:ARG:HE	2:I:163:VAL:HG11	1.83	0.42
2:K:146:VAL:HG12	2:K:196:VAL:HG22	2.01	0.42
2:I:54:ARG:NH2	6:I:410:HOH:O	2.52	0.42
1:F:30:ASN:HB2	6:F:440:HOH:O	2.19	0.42
1:G:6:GLU:CD	1:G:116:GLY:H	2.22	0.42
1:G:59:TYR:CD2	3:D:420:TRP:HZ3	2.36	0.42
1:G:136:PRO:HD3	1:G:148:LEU:HB3	2.01	0.42
2:K:149:LYS:HG3	2:K:193:ALA:HB3	2.00	0.42
1:G:35:HIS:CD2	1:G:110:PHE:HE2	2.38	0.42
2:J:125:LEU:HD21	2:J:186:TYR:CD2	2.55	0.42
1:F:173:VAL:HG12	1:F:192:VAL:HB	2.01	0.42
1:E:6:GLU:OE1	1:E:114:GLY:CA	2.60	0.41
1:E:126:THR:HG22	1:E:213:SER:HB2	2.02	0.41
1:G:36:TRP:NE1	1:G:81:LEU:HB2	2.35	0.41
2:J:115:VAL:O	2:J:116:PHE:HD1	2.03	0.41
1:G:122:SER:HB3	1:G:156:PHE:HZ	1.85	0.41
1:E:149:GLY:HA2	1:E:164:TRP:CH2	2.54	0.41
1:E:206:CYS:SG	1:E:219:LYS:HB3	2.61	0.41
2:I:193:ALA:HB1	2:I:206:THR:HG23	2.02	0.41
1:F:204:TYR:O	1:F:221:VAL:N	2.46	0.41
2:K:113:PRO:HD2	2:K:201:LEU:HD11	2.01	0.41
2:K:195:GLU:OE1	2:K:206:THR:HG23	2.20	0.41
2:L:158:ASN:OD1	2:L:158:ASN:N	2.53	0.41
6:F:407:HOH:O	2:J:169:LYS:NZ	2.53	0.41
2:J:142:ARG:HE	2:J:163:VAL:HG11	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:186:TYR:O	2:J:211:ARG:NH1	2.53	0.41
1:G:35:HIS:CD2	1:G:47:TRP:HE1	2.29	0.41
2:L:125:LEU:HA	2:L:125:LEU:HD23	1.77	0.41
1:E:34:MET:CB	1:E:79:LEU:HD13	2.51	0.41
1:E:152:VAL:N	1:E:188:LEU:O	2.41	0.41
1:E:215:THR:HG22	1:E:217:VAL:HG13	2.01	0.41
2:I:136:LEU:HB2	2:I:175:LEU:HB3	2.02	0.41
2:K:155:GLN:OE1	2:K:158:ASN:ND2	2.54	0.41
2:J:183:LYS:O	2:J:187:GLU:HG2	2.21	0.41
1:G:73:ASP:OD1	1:G:76:LYS:HG2	2.21	0.41
1:E:169:LEU:HD21	1:E:192:VAL:HG21	2.03	0.41
2:J:193:ALA:HB1	2:J:206:THR:CG2	2.51	0.41
2:K:197:THR:CG2	2:K:197:THR:O	2.69	0.41
2:I:94:TRP:C	2:I:96:ILE:HG13	2.41	0.41
2:J:142:ARG:HD2	2:J:173:TYR:CD1	2.56	0.41
2:J:193:ALA:HB2	2:J:208:SER:HB3	2.03	0.41
1:G:9:GLY:HA3	1:G:117:THR:HG22	2.03	0.41
2:K:19:ALA:O	2:K:74:THR:HA	2.20	0.41
2:K:207:LYS:HA	2:K:207:LYS:HE2	2.03	0.41
2:J:192:TYR:HB2	2:J:209:PHE:CZ	2.56	0.40
2:K:2:LEU:HD12	2:K:90:GLN:OE1	2.21	0.40
2:K:91:ARG:NH2	6:K:413:HOH:O	2.55	0.40
1:H:136:PRO:HG3	1:H:148:LEU:CD2	2.51	0.40
2:I:148:TRP:HE3	6:I:407:HOH:O	2.04	0.40
2:K:12:SER:O	2:K:13:LEU:HD23	2.21	0.40
1:F:114:GLY:O	2:J:43:ALA:HB2	2.21	0.40
1:E:129:PRO:CB	1:E:155:TYR:HB3	2.49	0.40
1:H:205:ILE:CD1	1:H:220:LYS:HG3	2.51	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	E	225/226 (100%)	212 (94%)	10 (4%)	3 (1%)	10	6
1	F	225/226 (100%)	216 (96%)	9 (4%)	0	100	100
1	G	225/226 (100%)	216 (96%)	9 (4%)	0	100	100
1	H	226/226 (100%)	217 (96%)	9 (4%)	0	100	100
2	I	214/213 (100%)	207 (97%)	7 (3%)	0	100	100
2	J	214/213 (100%)	205 (96%)	8 (4%)	1 (0%)	25	25
2	K	210/213 (99%)	199 (95%)	10 (5%)	1 (0%)	25	25
2	L	213/213 (100%)	208 (98%)	5 (2%)	0	100	100
3	A	13/15 (87%)	13 (100%)	0	0	100	100
3	B	14/15 (93%)	14 (100%)	0	0	100	100
3	C	14/15 (93%)	12 (86%)	2 (14%)	0	100	100
3	D	13/15 (87%)	13 (100%)	0	0	100	100
All	All	1806/1816 (99%)	1732 (96%)	69 (4%)	5 (0%)	37	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	64	VAL
1	E	214	ASN
2	K	30	SER
2	J	210	ASN
1	E	212	PRO

### 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	E	194/195 (100%)	190 (98%)	4 (2%)	48	57
1	F	196/195 (100%)	193 (98%)	3 (2%)	60	70
1	G	195/195 (100%)	191 (98%)	4 (2%)	48	57
1	H	197/195 (101%)	195 (99%)	2 (1%)	73	80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	188/185 (102%)	183 (97%)	5 (3%)	40	48
2	J	188/185 (102%)	182 (97%)	6 (3%)	34	42
2	K	182/185 (98%)	175 (96%)	7 (4%)	28	34
2	L	187/185 (101%)	184 (98%)	3 (2%)	58	69
3	A	14/14 (100%)	14 (100%)	0	100	100
3	B	15/14 (107%)	15 (100%)	0	100	100
3	C	15/14 (107%)	15 (100%)	0	100	100
3	D	14/14 (100%)	14 (100%)	0	100	100
All	All	1585/1576 (101%)	1551 (98%)	34 (2%)	48	57

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	30[A]	ASN
1	H	30[B]	ASN
2	L	33	LEU
2	L	90	GLN
2	L	91	ARG
1	E	19	ARG
1	E	127	LYS
1	E	171	SER
1	E	180	LEU
2	I	33	LEU
2	I	69	THR
2	I	91	ARG
2	I	149	LYS
2	I	154	LEU
1	F	148	LEU
1	F	185	LEU
1	F	219	LYS
2	J	54	ARG
2	J	91	ARG
2	J	140	TYR
2	J	149	LYS
2	J	164	THR
2	J	190	LYS
1	G	5	LEU
1	G	30	ASN
1	G	188	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	207	ASN
2	K	67	SER
2	K	91	ARG
2	K	154	LEU
2	K	177	ASN
2	K	185	ASP
2	K	210	ASN
2	K	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	147	GLN
2	L	177	ASN
1	E	174	HIS
1	E	181	GLN
1	E	210	HIS
2	I	166	GLN
3	B	412	GLN
1	F	174	HIS
1	F	209	ASN
2	J	6	GLN
2	J	137	ASN
2	J	155	GLN
1	G	35	HIS
2	K	152	ASN
2	K	177	ASN
2	K	199	GLN
2	K	210	ASN

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 21 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ACT	F	301	-	3,3,3	0.60	0	3,3,3	1.57	1 (33%)
4	ACT	E	301	-	3,3,3	0.99	0	3,3,3	1.21	0
4	ACT	G	301	-	3,3,3	1.13	0	3,3,3	1.48	1 (33%)
4	ACT	H	301	-	3,3,3	0.71	0	3,3,3	1.04	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	G	301	ACT	OXT-C-O	-2.09	114.26	122.03
4	F	301	ACT	OXT-C-CH3	2.02	123.54	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	301	ACT	2	0
4	E	301	ACT	7	0
4	G	301	ACT	2	0
4	H	301	ACT	1	0

## 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	E	226/226 (100%)	1.76	101 (44%) <b>1</b> <b>0</b>	26, 116, 200, 238	1 (0%)
1	F	226/226 (100%)	0.76	45 (19%) <b>3</b> <b>3</b>	24, 58, 179, 230	1 (0%)
1	G	226/226 (100%)	0.97	40 (17%) <b>4</b> <b>4</b>	37, 68, 138, 213	1 (0%)
1	H	226/226 (100%)	0.17	14 (6%) <b>28</b> <b>27</b>	21, 49, 128, 170	2 (0%)
2	I	212/213 (99%)	0.91	50 (23%) <b>2</b> <b>2</b>	28, 75, 191, 220	4 (1%)
2	J	212/213 (99%)	0.83	48 (22%) <b>3</b> <b>3</b>	21, 62, 151, 171	4 (1%)
2	K	211/213 (99%)	0.95	27 (12%) <b>9</b> <b>8</b>	40, 73, 122, 152	1 (0%)
2	L	212/213 (99%)	0.15	9 (4%) <b>41</b> <b>41</b>	16, 48, 120, 138	3 (1%)
3	A	15/15 (100%)	-0.47	0 <b>100</b> <b>100</b>	30, 38, 45, 52	0
3	B	15/15 (100%)	-0.18	0 <b>100</b> <b>100</b>	23, 43, 53, 58	1 (6%)
3	C	15/15 (100%)	-0.04	0 <b>100</b> <b>100</b>	28, 41, 59, 72	1 (6%)
3	D	15/15 (100%)	0.22	0 <b>100</b> <b>100</b>	50, 63, 71, 71	0
All	All	1811/1816 (99%)	0.79	334 (18%) <b>4</b> <b>4</b>	16, 66, 171, 238	19 (1%)

All (334) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	168	ALA	5.7
1	G	11	VAL	5.6
1	E	152	VAL	5.2
1	F	172	GLY	5.2
1	G	199	LEU	5.2
1	E	160	VAL	5.1
2	J	186	TYR	5.0
1	E	134	LEU	4.8
1	E	205	ILE	4.8
1	E	133	PRO	4.6
1	E	150	CYS	4.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	I	184	ALA	4.4
2	I	192	TYR	4.4
2	I	178	THR	4.4
1	E	169	LEU	4.3
2	I	180	THR	4.3
1	F	137	SER	4.2
1	E	162	VAL	4.2
1	E	212	PRO	4.2
1	E	68	PHE	4.1
1	F	208	VAL	4.1
2	I	181	LEU	4.0
2	J	142	ARG	4.0
1	E	135	ALA	4.0
1	F	147	ALA	4.0
2	K	154	LEU	4.0
2	I	133	VAL	3.9
2	J	132	VAL	3.9
1	G	15	GLY	3.9
1	E	146	ALA	3.9
1	E	151	LEU	3.9
2	I	119	PRO	3.9
1	E	204	TYR	3.9
1	F	204	TYR	3.9
1	G	224	LYS	3.8
1	E	199	LEU	3.8
1	F	199	LEU	3.8
1	F	191	VAL	3.8
2	J	135	LEU	3.8
2	I	116	PHE	3.8
2	J	181	LEU	3.7
2	K	73	LEU	3.7
2	I	118	PHE	3.7
1	E	64	VAL	3.7
1	F	193	THR	3.7
1	F	194	VAL	3.7
1	E	226	CYS	3.7
2	I	154	LEU	3.7
2	J	116	PHE	3.7
2	J	117	ILE	3.6
1	E	208	VAL	3.6
1	E	15	GLY	3.6
2	J	150	VAL	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	217	VAL	3.5
2	I	114[A]	SER	3.5
1	E	143	GLY	3.5
1	F	150	CYS	3.5
2	J	209	PHE	3.5
2	J	115	VAL	3.5
2	I	136	LEU	3.5
2	K	27	GLN	3.5
2	J	144	ALA	3.5
1	E	18	LEU	3.4
1	G	143	GLY	3.4
1	E	186	TYR	3.4
1	E	192	VAL	3.4
2	I	194	CYS	3.4
1	F	169	LEU	3.4
1	G	226	CYS	3.3
1	H	143	GLY	3.3
2	J	205	VAL	3.3
1	F	205	ILE	3.3
1	G	201	THR	3.3
1	E	157	PRO	3.3
2	J	196	VAL	3.3
1	E	178	ALA	3.3
1	F	192	VAL	3.2
1	E	209	ASN	3.2
1	H	138	SER	3.2
1	E	148	LEU	3.2
1	E	175	THR	3.2
1	E	132	PHE	3.2
1	G	142	SER	3.2
1	F	226	CYS	3.2
1	G	197	SER	3.1
2	I	186	TYR	3.1
1	E	215	THR	3.1
1	F	145	THR	3.1
2	J	118	PHE	3.1
2	I	148	TRP	3.1
2	J	140	TYR	3.1
1	G	195	PRO	3.1
2	L	181	LEU	3.1
1	G	17	SER	3.1
1	E	121	VAL	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	J	148	TRP	3.1
1	E	141	THR	3.1
1	H	169	LEU	3.0
2	J	212	GLY	3.0
2	K	28	SER	3.0
1	E	191	VAL	3.0
1	E	147	ALA	3.0
2	K	24	ARG	3.0
1	E	149	GLY	3.0
1	F	188	LEU	3.0
2	K	2	LEU	3.0
2	K	201	LEU	3.0
2	L	213	GLU	3.0
1	E	11	VAL	3.0
2	J	133	VAL	3.0
1	G	145	THR	3.0
1	E	140	SER	3.0
2	I	182	SER	3.0
2	J	139	PHE	3.0
1	E	173	VAL	3.0
1	G	198	SER	2.9
1	E	206	CYS	2.9
2	I	120	PRO	2.9
2	I	212	GLY	2.9
2	K	191	VAL	2.9
1	F	146	ALA	2.9
1	G	146	ALA	2.9
1	F	135	ALA	2.9
1	F	201	THR	2.9
2	J	109	THR	2.9
1	F	149	GLY	2.9
1	G	200	GLY	2.9
1	E	86	LEU	2.9
1	E	188	LEU	2.9
1	F	151	LEU	2.9
1	E	164	TRP	2.8
2	I	205	VAL	2.8
2	I	197	THR	2.8
2	L	212	GLY	2.8
1	F	134	LEU	2.8
1	H	140	SER	2.8
2	K	205	VAL	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	K	68	GLY	2.8
1	E	165	ASN	2.8
1	H	137	SER	2.8
1	E	142	SER	2.8
2	I	196	VAL	2.8
2	K	197	THR	2.8
1	G	18	LEU	2.8
2	J	149	LYS	2.8
2	K	196	VAL	2.8
2	K	192	TYR	2.7
1	E	194	VAL	2.7
1	F	173	VAL	2.7
2	I	191	VAL	2.7
1	E	130	SER	2.7
1	F	129	PRO	2.7
2	I	146	VAL	2.7
2	I	150	VAL	2.7
1	E	174	HIS	2.7
1	E	79	LEU	2.7
1	E	83	MET	2.7
1	G	14	PRO	2.7
2	J	141	PRO	2.7
2	I	115	VAL	2.7
1	H	224	LYS	2.7
1	E	161	THR	2.7
1	E	180	LEU	2.7
1	F	170	THR	2.7
1	F	136	PRO	2.7
1	E	12	VAL	2.7
2	K	149	LYS	2.7
1	E	167	GLY	2.6
1	E	17	SER	2.6
1	E	183	SER	2.6
1	E	223	PRO	2.6
1	E	155	TYR	2.6
2	I	206	THR	2.6
1	E	197	SER	2.6
2	I	127	SER	2.6
1	F	216	LYS	2.6
2	J	110	VAL	2.6
1	G	117	THR	2.6
2	J	154	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	I	159	SER	2.6
1	E	220	LYS	2.6
1	G	13	GLN	2.6
1	G	144	GLY	2.6
2	K	153	ALA	2.6
1	E	224	LYS	2.6
2	I	145	LYS	2.6
1	E	67	ARG	2.6
1	E	131	VAL	2.5
1	E	156	PHE	2.5
2	I	179	LEU	2.5
2	J	189	HIS	2.5
1	H	13	GLN	2.5
1	E	128	GLY	2.5
2	L	191	VAL	2.5
2	J	192	TYR	2.5
1	E	210	HIS	2.5
2	J	111	ALA	2.5
2	L	210	ASN	2.5
1	E	179	VAL	2.5
2	J	131	SER	2.4
1	F	143	GLY	2.4
2	J	207	LYS	2.4
2	I	144	ALA	2.4
1	G	16	ARG	2.4
2	I	177	ASN	2.4
1	F	138	SER	2.4
1	E	218	ASP	2.4
1	E	66	GLY	2.4
1	F	131	VAL	2.4
1	E	200	GLY	2.4
1	G	86	LEU	2.4
2	K	184	ALA	2.4
1	E	217	VAL	2.4
1	E	201	THR	2.4
1	H	198	SER	2.4
1	E	85	SER	2.4
1	E	124	ALA	2.4
2	L	150	VAL	2.3
1	E	88	THR	2.3
1	E	91	THR	2.3
1	F	164	TRP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	J	120	PRO	2.3
1	E	87	LYS	2.3
1	E	189	SER	2.3
1	F	148	LEU	2.3
2	K	180	THR	2.3
1	G	59	TYR	2.3
2	J	136	LEU	2.3
1	G	61	ALA	2.3
1	G	168	ALA	2.3
2	K	207	LYS	2.3
1	E	136	PRO	2.3
1	G	12	VAL	2.3
2	L	129	THR	2.3
2	I	125	LEU	2.3
1	F	203	THR	2.3
1	F	183	SER	2.3
1	F	225	SER	2.3
2	I	131	SER	2.3
1	F	200	GLY	2.3
2	I	128	GLY	2.3
2	J	188	LYS	2.2
1	G	204	TYR	2.2
1	H	199	LEU	2.2
1	E	20	LEU	2.2
2	I	164	THR	2.2
2	K	29	VAL	2.2
1	E	63	SER	2.2
1	E	222	GLU	2.2
1	G	5	LEU	2.2
2	I	152	ASN	2.2
2	J	179	LEU	2.2
2	K	137	ASN	2.2
2	I	204	PRO	2.2
1	E	69	THR	2.2
1	E	145	THR	2.2
2	J	191	VAL	2.2
1	E	153	LYS	2.2
2	I	149	LYS	2.2
2	K	190	LYS	2.2
2	I	200	GLY	2.2
2	J	130	ALA	2.2
1	G	141	THR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	J	206	THR	2.2
2	K	3	THR	2.2
1	E	190	SER	2.2
2	K	26	SER	2.2
1	G	205	ILE	2.2
1	E	120	THR	2.2
2	J	129	THR	2.2
2	I	209	PHE	2.2
1	E	138	SER	2.1
1	G	196	SER	2.1
2	I	134	CYS	2.1
2	I	171	SER	2.1
2	J	187	GLU	2.1
2	J	194	CYS	2.1
1	G	67	ARG	2.1
2	J	201	LEU	2.1
1	E	14	PRO	2.1
1	G	223	PRO	2.1
1	E	13	GLN	2.1
1	G	202	GLN	2.1
2	J	193	ALA	2.1
1	H	126	THR	2.1
2	I	190	LYS	2.1
1	H	142	SER	2.1
1	E	198	SER	2.1
1	G	138	SER	2.1
1	E	207	ASN	2.1
1	F	214	ASN	2.1
2	J	190	LYS	2.1
1	G	121	VAL	2.1
2	J	146	VAL	2.1
1	F	132	PHE	2.1
2	I	139	PHE	2.1
1	G	85	SER	2.1
1	G	225	SER	2.1
2	I	201	LEU	2.1
1	E	129	PRO	2.1
1	F	139	LYS	2.1
2	J	169	LYS	2.1
1	E	203	THR	2.1
1	E	125	SER	2.1
1	E	184	GLY	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	225	SER	2.1
2	I	203	SER	2.1
2	K	194	CYS	2.1
1	E	82	GLN	2.1
1	F	133	PRO	2.1
2	I	137	ASN	2.1
1	H	141	THR	2.1
1	H	145	THR	2.1
1	G	203	THR	2.1
2	L	180	THR	2.1
2	K	69	THR	2.1
1	H	194	VAL	2.0
1	F	152	VAL	2.0
2	K	71	PHE	2.0
1	E	144	GLY	2.0
2	J	126	LYS	2.0
1	E	159	PRO	2.0
2	J	113	PRO	2.0
2	J	119	PRO	2.0
2	K	152	ASN	2.0
2	I	193	ALA	2.0
2	J	180	THR	2.0
1	F	144	GLY	2.0
2	L	209	PHE	2.0
1	F	163	SER	2.0
1	F	189	SER	2.0
1	E	70	ILE	2.0
2	I	117	ILE	2.0
1	G	84	ASN	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 ⓘ

There are no monosaccharides in this entry.



## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	CA	G	303	1/1	0.53	0.18	120,120,120,120	0
5	CA	K	304	1/1	0.66	0.24	110,110,110,110	0
5	CA	J	302	1/1	0.79	0.19	142,142,142,142	0
5	CA	K	303	1/1	0.84	0.17	114,114,114,114	0
4	ACT	E	301	4/4	0.84	0.12	39,46,48,57	0
5	CA	K	305	1/1	0.84	0.23	98,98,98,98	0
5	CA	C	501	1/1	0.87	0.21	103,103,103,103	0
5	CA	A	501	1/1	0.88	0.19	117,117,117,117	0
5	CA	K	302	1/1	0.89	0.11	96,96,96,96	0
5	CA	L	301	1/1	0.90	0.14	89,89,89,89	0
5	CA	H	302	1/1	0.91	0.08	75,75,75,75	0
4	ACT	H	301	4/4	0.91	0.12	44,44,47,48	0
4	ACT	G	301	4/4	0.92	0.09	36,44,47,54	0
5	CA	J	301	1/1	0.93	0.07	76,76,76,76	0
4	ACT	F	301	4/4	0.93	0.10	36,42,45,48	0
5	CA	F	303	1/1	0.94	0.08	97,97,97,97	0
5	CA	G	302	1/1	0.94	0.07	86,86,86,86	0
5	CA	F	305	1/1	0.94	0.13	80,80,80,80	0
5	CA	K	301	1/1	0.94	0.12	101,101,101,101	0
5	CA	F	304	1/1	0.96	0.07	74,74,74,74	0
5	CA	F	302	1/1	0.96	0.08	81,81,81,81	0
5	CA	E	302	1/1	0.96	0.07	75,75,75,75	0
5	CA	H	303	1/1	0.97	0.07	65,65,65,65	0
5	CA	L	302	1/1	0.99	0.05	60,60,60,60	0
5	CA	I	301	1/1	0.99	0.05	64,64,64,64	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.