



# wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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

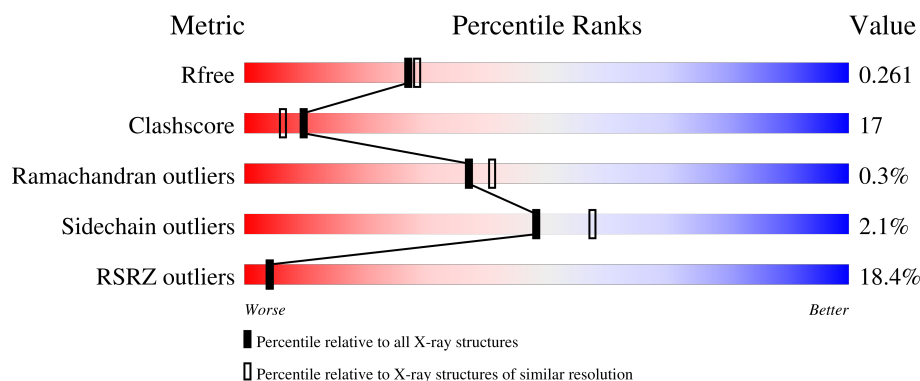
# 1 Overall quality at a glance

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			

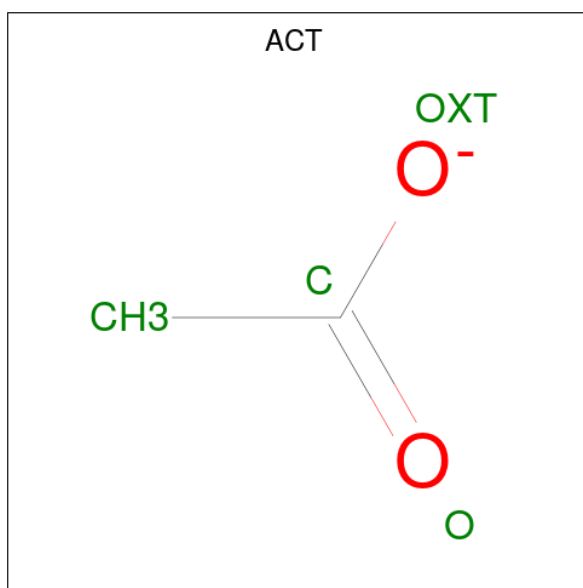
- Molecule 2 is a protein called HCV1-C1 Antibody Fab Light Chain.

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

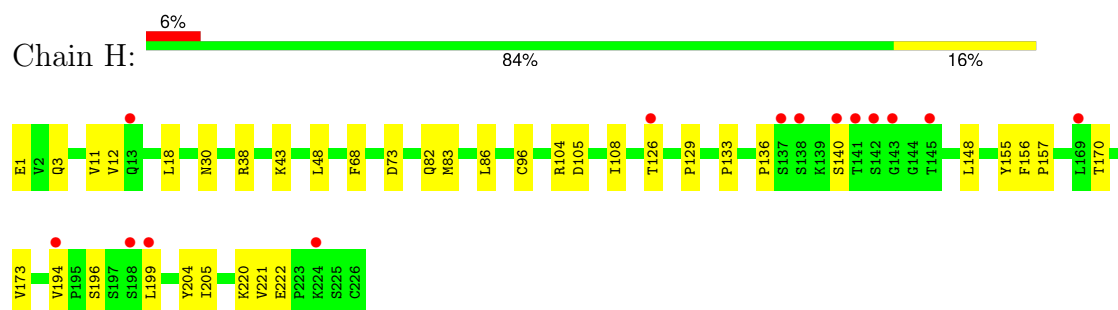
- Molecule 6 is water.

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

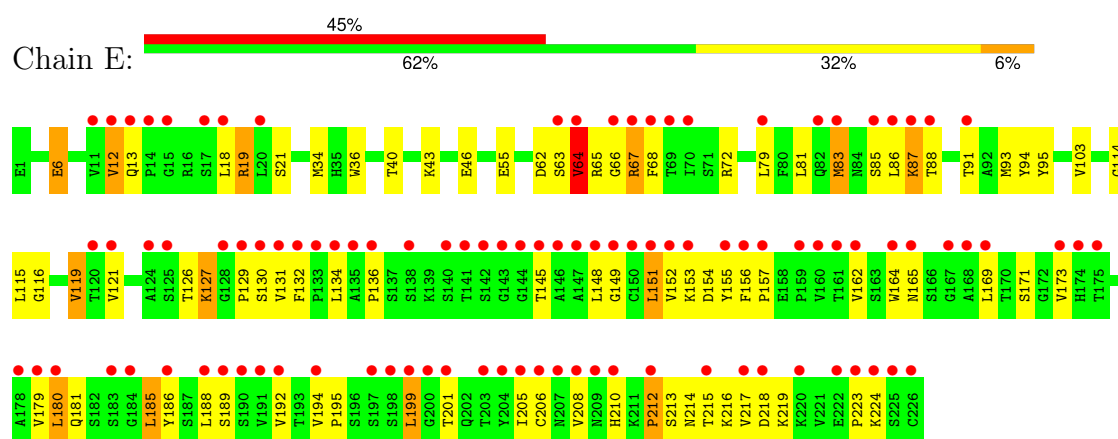
### 3 Residue-property plots [i](#)

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.

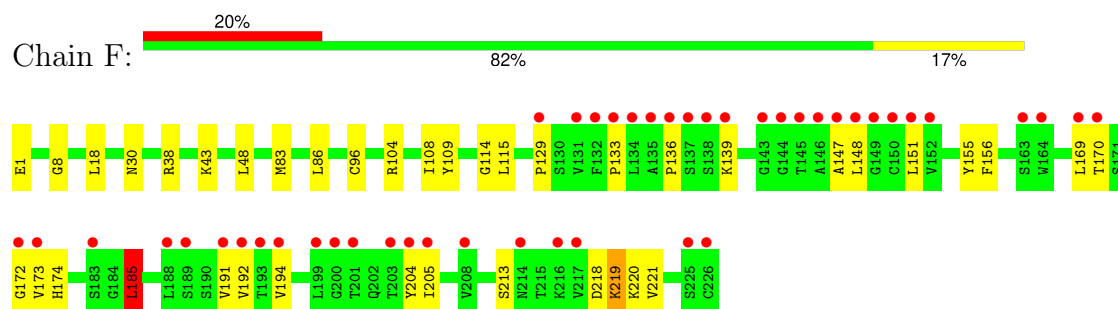
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



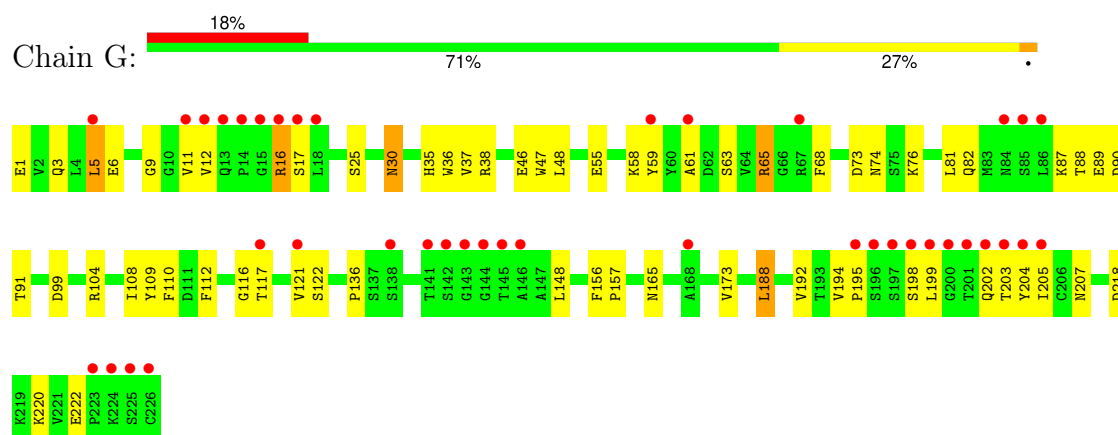
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



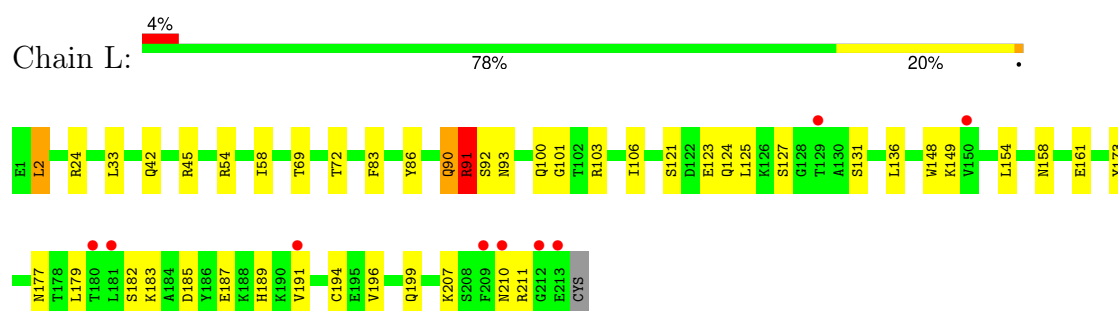
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



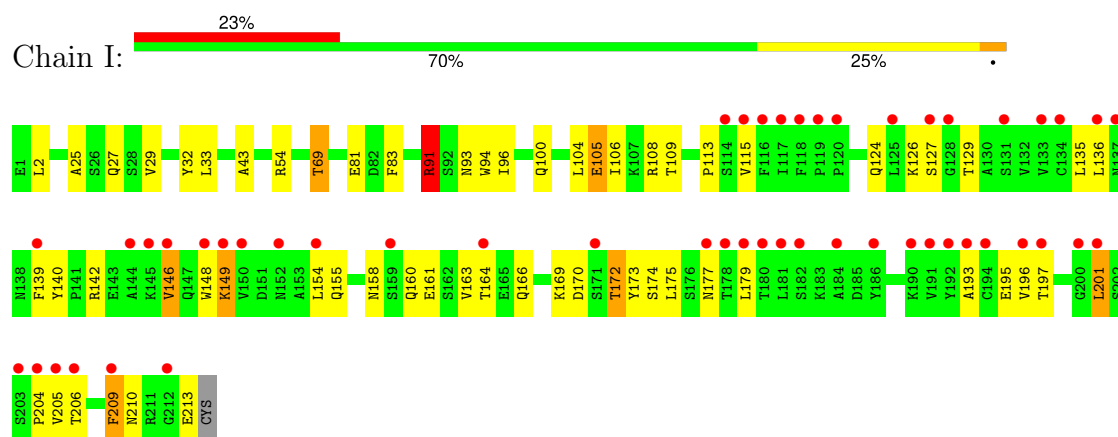
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



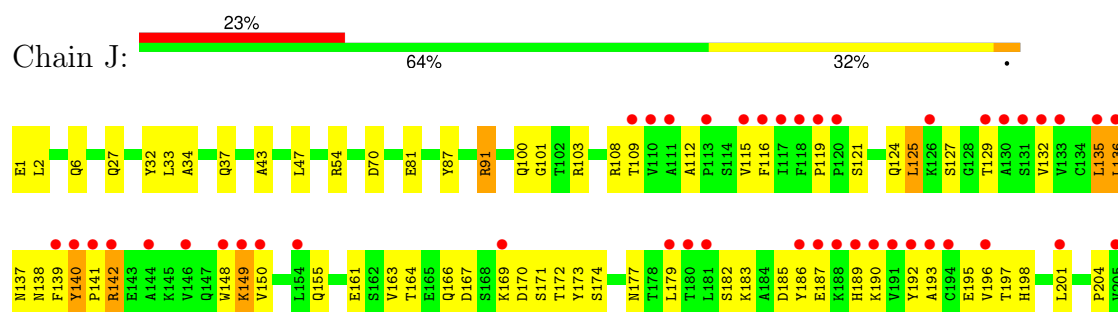
• Molecule 2: HCV1-C1 Antibody Fab Light Chain



• Molecule 2: HCV1-C1 Antibody Fab Light Chain



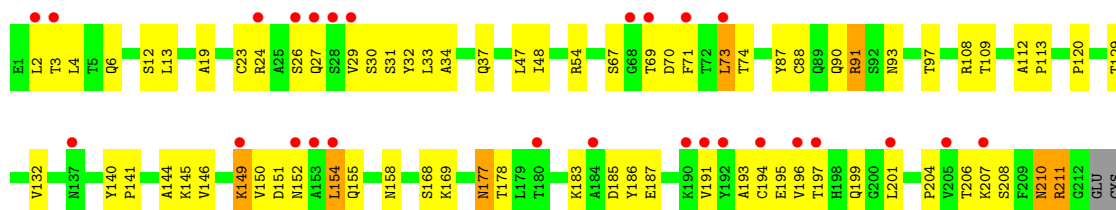
• Molecule 2: HCV1-C1 Antibody Fab Light Chain



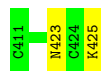
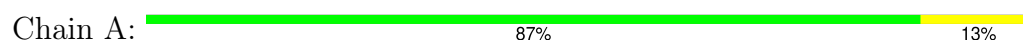




• Molecule 2: HCV1-C1 Antibody Fab Light Chain



• 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

The worst 5 of 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

The worst 5 of 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

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
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

*Continued on next page...*

*Continued from previous page...*

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

The worst 5 of 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
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

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	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
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

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	91	ARG
2	K	154	LEU
2	K	210	ASN
2	I	149	LYS
2	I	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	177	ASN
2	K	210	ASN
1	F	174	HIS
1	F	209	ASN
2	J	6	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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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(°)	Ideal(°)
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

The worst 5 of 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

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

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 [i](#)

There are no such residues in this entry.