



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:14 PM GMT

PDB ID : 4XGZ  
Title : Crystal structure of human paxillin LD2 motif in complex with Fab fragment  
Authors : Nocula-Lugowska, M.; Lugowski, M.; Salgia, R.; Kossiakoff, A.A.  
Deposited on : 2015-01-04  
Resolution : 2.50 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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-20026982

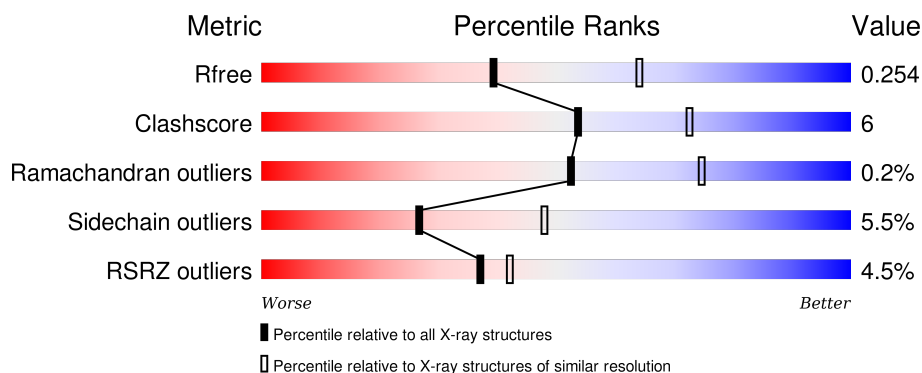
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	229	<div> <div></div> <div>86% 9% 5%</div> </div>
1	C	229	<div> <div>%</div> <div>84% 10% . .</div> </div>
1	E	229	<div> <div>13%</div> <div>83% 9% 7%</div> </div>
1	G	229	<div> <div>2%</div> <div>86% 8% . 5%</div> </div>
1	H	229	<div> <div></div> <div>85% 9% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	J	229	
1	M	229	
1	O	229	
1	Q	229	
1	S	229	
1	U	229	
1	W	229	
2	B	215	
2	D	215	
2	F	215	
2	I	215	
2	K	215	
2	L	215	
2	N	215	
2	P	215	
2	R	215	
2	T	215	
2	V	215	
2	X	215	
3	a	19	
3	c	19	
3	e	19	
3	g	19	
3	h	19	
3	j	19	

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Mol	Chain	Length	Quality of chain
3	m	19	
3	o	19	
3	q	19	
3	s	19	
3	u	19	
3	w	19	

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	NO3	B	301	-	-	-	X
4	NO3	D	301	-	-	-	X
4	NO3	F	301	-	-	-	X
4	NO3	K	301	-	-	-	X
4	NO3	L	301	-	-	-	X
4	NO3	P	301	-	-	-	X
4	NO3	T	301	-	-	-	X
4	NO3	V	301	-	-	-	X
5	EDO	Q	301	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 40426 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 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1620	1027	266	320	7			
1	C	219	Total	C	N	O	S	0	0	0
			1633	1034	268	324	7			
1	E	212	Total	C	N	O	S	0	0	0
			1586	1009	260	311	6			
1	G	218	Total	C	N	O	S	0	0	0
			1624	1029	267	321	7			
1	H	219	Total	C	N	O	S	0	0	0
			1634	1036	269	323	6			
1	J	224	Total	C	N	O	S	0	0	0
			1662	1051	273	331	7			
1	M	220	Total	C	N	O	S	0	0	0
			1643	1040	270	326	7			
1	O	223	Total	C	N	O	S	0	0	0
			1660	1049	273	331	7			
1	Q	217	Total	C	N	O	S	0	0	0
			1618	1025	265	321	7			
1	S	215	Total	C	N	O	S	0	0	0
			1612	1025	264	317	6			
1	U	217	Total	C	N	O	S	0	0	0
			1618	1026	266	319	7			
1	W	218	Total	C	N	O	S	0	0	0
			1624	1029	267	321	7			

- Molecule 2 is a protein called FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1593	992	269	327	5			
2	D	210	Total	C	N	O	S	0	0	0
			1593	992	269	327	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	207	Total	C	N	O	S	0	0	0
			1568	979	263	322	4			
2	I	211	Total	C	N	O	S	0	0	0
			1598	995	270	328	5			
2	K	210	Total	C	N	O	S	0	0	0
			1593	992	269	327	5			
2	L	209	Total	C	N	O	S	0	0	0
			1587	989	268	326	4			
2	N	210	Total	C	N	O	S	0	0	0
			1593	992	269	327	5			
2	P	210	Total	C	N	O	S	0	0	0
			1593	992	269	327	5			
2	R	211	Total	C	N	O	S	0	0	0
			1601	997	270	328	6			
2	T	210	Total	C	N	O	S	0	0	0
			1593	992	269	327	5			
2	V	210	Total	C	N	O	S	0	0	0
			1593	992	269	327	5			
2	X	210	Total	C	N	O	S	0	0	0
			1593	992	269	327	5			

- Molecule 3 is a protein called PAXILLIN LD2.

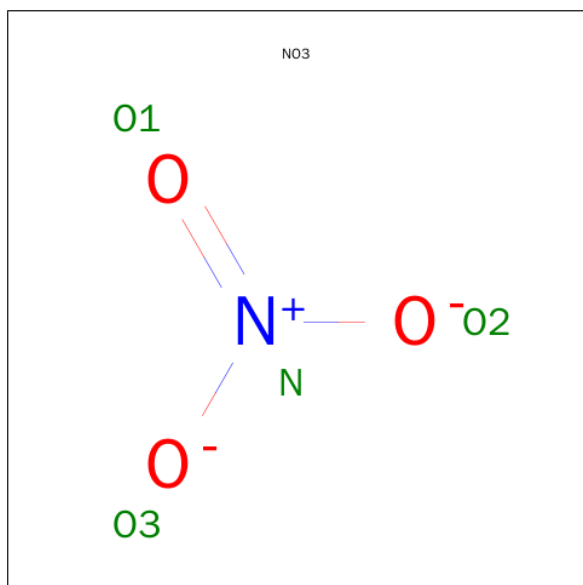
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	a	12	Total	C	N	O	0	0	0
			99	63	16	20			
3	c	16	Total	C	N	O	0	0	0
			128	80	22	26			
3	e	13	Total	C	N	O	0	0	0
			107	67	18	22			
3	g	13	Total	C	N	O	0	0	0
			107	67	18	22			
3	h	12	Total	C	N	O	0	0	0
			99	63	16	20			
3	j	19	Total	C	N	O	0	0	0
			153	95	28	30			
3	m	13	Total	C	N	O	0	0	0
			107	67	18	22			
3	o	12	Total	C	N	O	0	0	0
			99	63	16	20			
3	q	19	Total	C	N	O	0	0	0
			153	95	28	30			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	s	12	Total	C	N	O	0	0	0
			99	63	16	20			
3	u	13	Total	C	N	O	0	0	0
			107	67	18	22			
3	w	12	Total	C	N	O	0	0	0
			99	63	16	20			

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



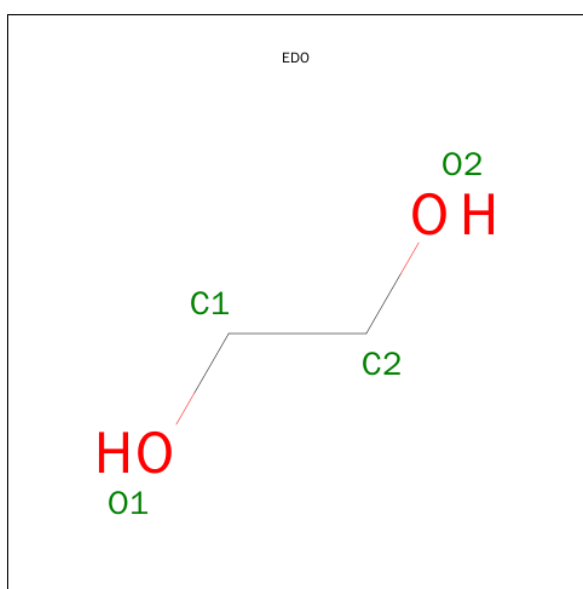
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	N	O	0	0
			4	1	3		
4	D	1	Total	N	O	0	0
			4	1	3		
4	F	1	Total	N	O	0	0
			4	1	3		
4	I	1	Total	N	O	0	0
			4	1	3		
4	K	1	Total	N	O	0	0
			4	1	3		
4	L	1	Total	N	O	0	0
			4	1	3		
4	N	1	Total	N	O	0	0
			4	1	3		
4	P	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	R	1	Total	N	O	0	0
			4	1	3		
4	T	1	Total	N	O	0	0
			4	1	3		
4	V	1	Total	N	O	0	0
			4	1	3		
4	X	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	C	O	0	0
			4	2	2		
5	Q	1	Total	C	O	0	0
			4	2	2		
5	W	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	B	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	19	Total O 19 19	0	0
6	D	16	Total O 16 16	0	0
6	E	10	Total O 10 10	0	0
6	F	2	Total O 2 2	0	0
6	G	19	Total O 19 19	0	0
6	H	29	Total O 29 29	0	0
6	I	14	Total O 14 14	0	0
6	J	17	Total O 17 17	0	0
6	K	13	Total O 13 13	0	0
6	L	17	Total O 17 17	0	0
6	M	25	Total O 25 25	0	0
6	N	31	Total O 31 31	0	0
6	O	13	Total O 13 13	0	0
6	P	11	Total O 11 11	0	0
6	Q	21	Total O 21 21	0	0
6	R	20	Total O 20 20	0	0
6	S	19	Total O 19 19	0	0
6	T	10	Total O 10 10	0	0
6	U	10	Total O 10 10	0	0
6	V	4	Total O 4 4	0	0
6	W	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	X	12	Total 12	O 12	0	0
6	a	1	Total 1	O 1	0	0
6	c	1	Total 1	O 1	0	0
6	e	1	Total 1	O 1	0	0
6	g	2	Total 2	O 2	0	0
6	j	4	Total 4	O 4	0	0
6	m	1	Total 1	O 1	0	0
6	o	1	Total 1	O 1	0	0
6	q	3	Total 3	O 3	0	0
6	s	1	Total 1	O 1	0	0
6	u	1	Total 1	O 1	0	0
6	w	1	Total 1	O 1	0	0

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


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

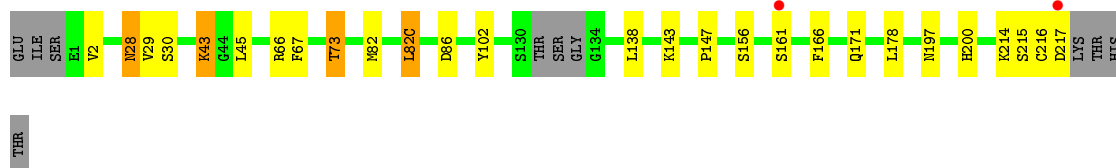
#### • Molecule 1: FAB HEAVY CHAIN

Chain A: 




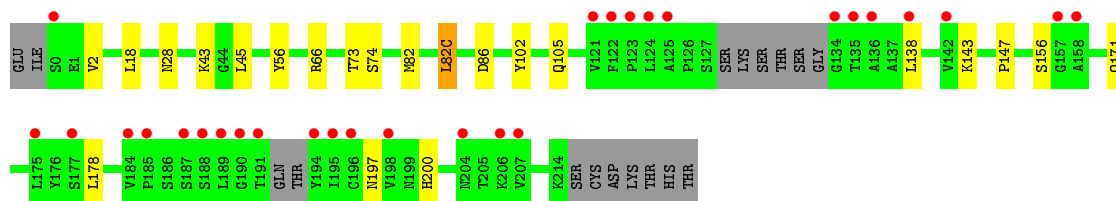
#### • Molecule 1: FAB HEAVY CHAIN

Chain C: 




#### • Molecule 1: FAB HEAVY CHAIN

Chain E: 




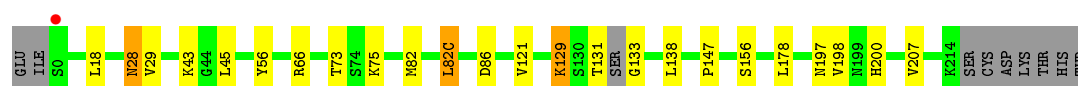
#### • Molecule 1: FAB HEAVY CHAIN

Chain G: 

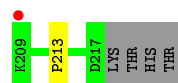
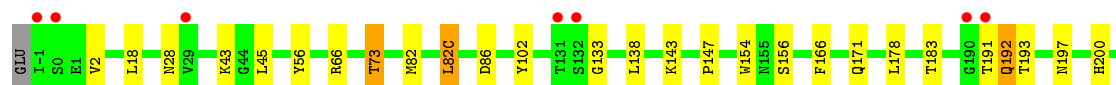
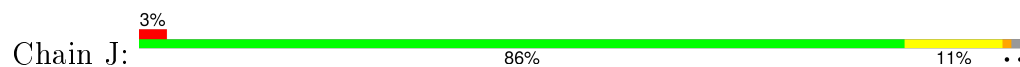


#### • Molecule 1: FAB HEAVY CHAIN

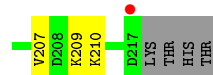
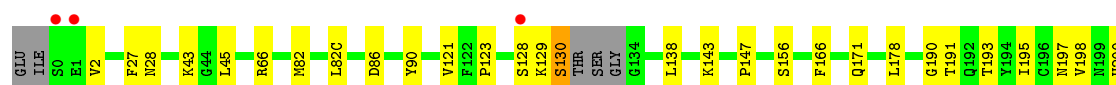
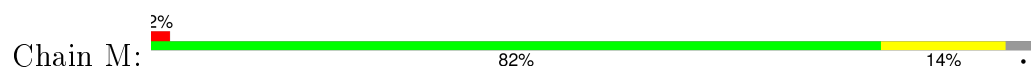
Chain H: 



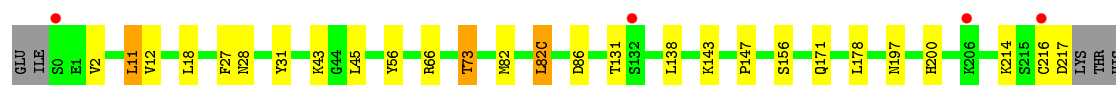
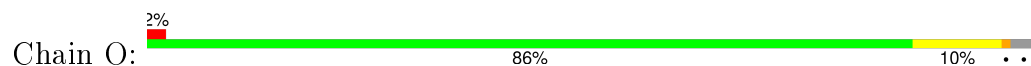
• Molecule 1: FAB HEAVY CHAIN



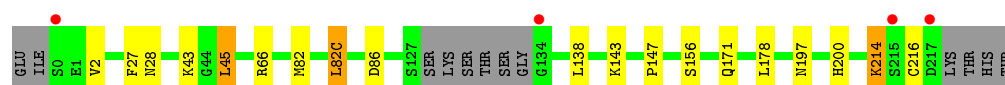
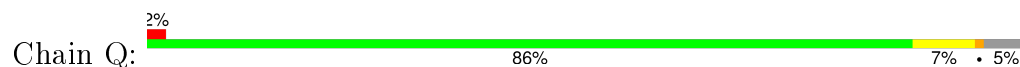
• Molecule 1: FAB HEAVY CHAIN



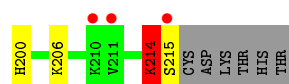
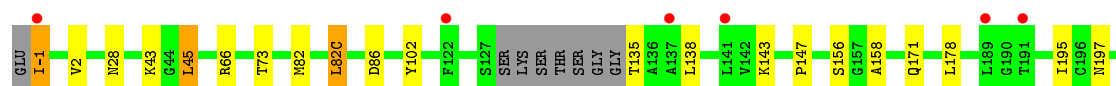
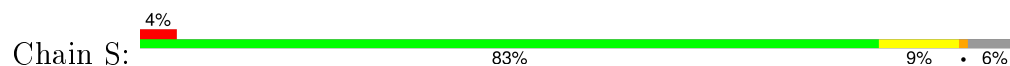
• Molecule 1: FAB HEAVY CHAIN



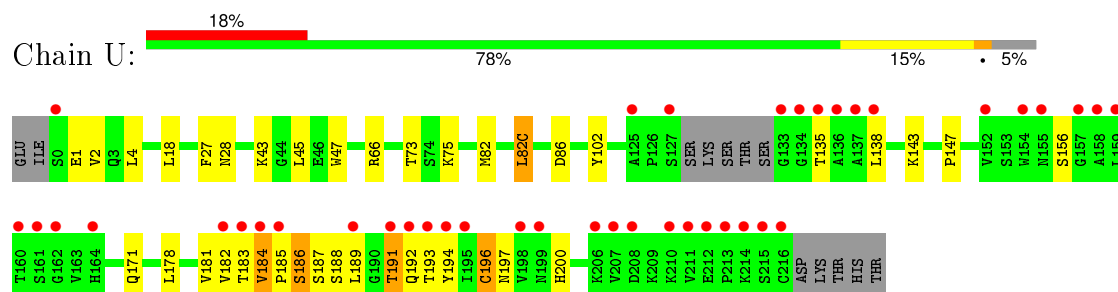
• Molecule 1: FAB HEAVY CHAIN



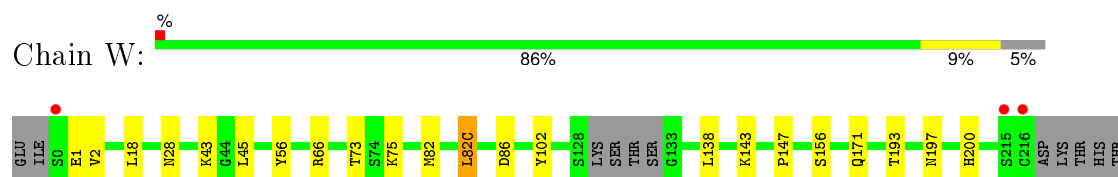
• Molecule 1: FAB HEAVY CHAIN



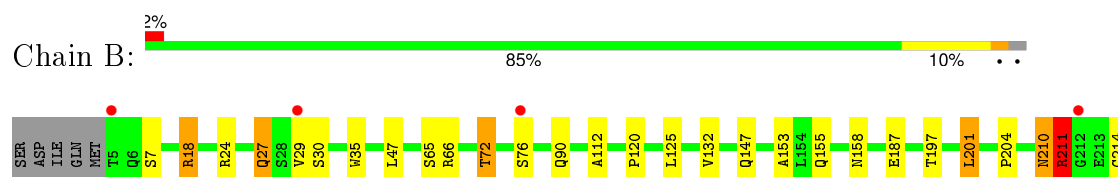
- Molecule 1: FAB HEAVY CHAIN



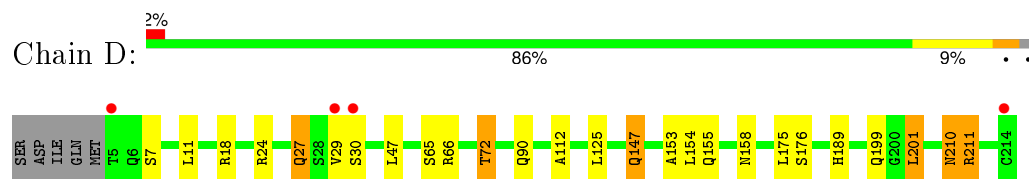
- Molecule 1: FAB HEAVY CHAIN



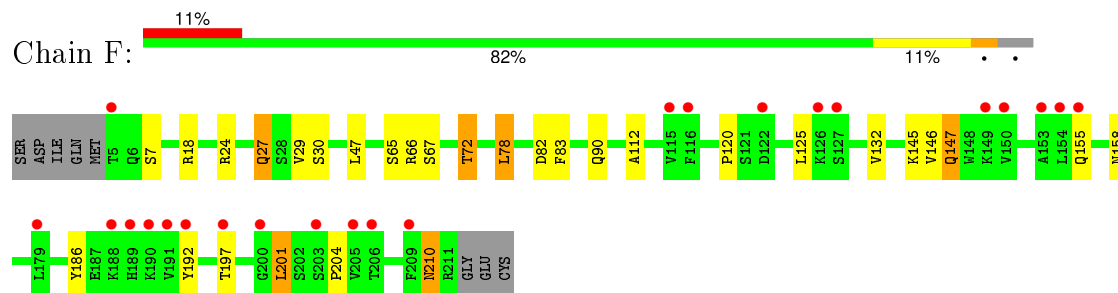
- Molecule 2: FAB LIGHT CHAIN



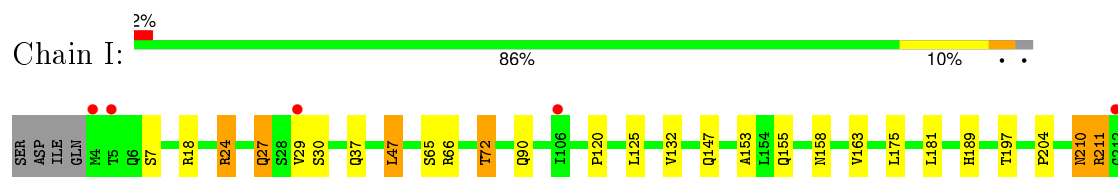
- Molecule 2: FAB LIGHT CHAIN



- Molecule 2: FAB LIGHT CHAIN



- Molecule 2: FAB LIGHT CHAIN





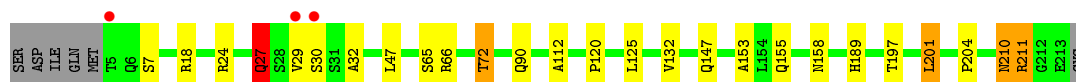
• Molecule 2: FAB LIGHT CHAIN

Chain K: 85% 11% ..



• Molecule 2: FAB LIGHT CHAIN

Chain L: 85% 10% ..



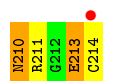
• Molecule 2: FAB LIGHT CHAIN

Chain N: 81% 13% ..



• Molecule 2: FAB LIGHT CHAIN

Chain P: 83% 12% ..



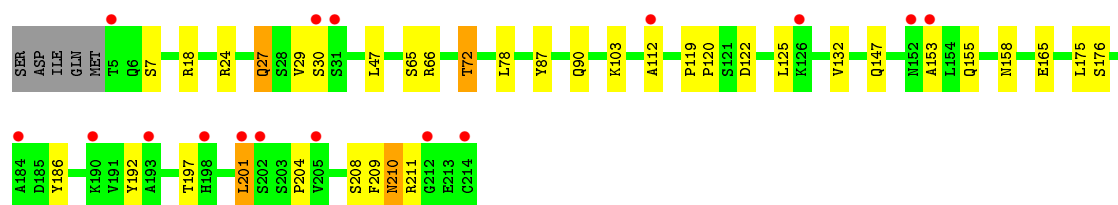
• Molecule 2: FAB LIGHT CHAIN

Chain R: 80% 16% ..

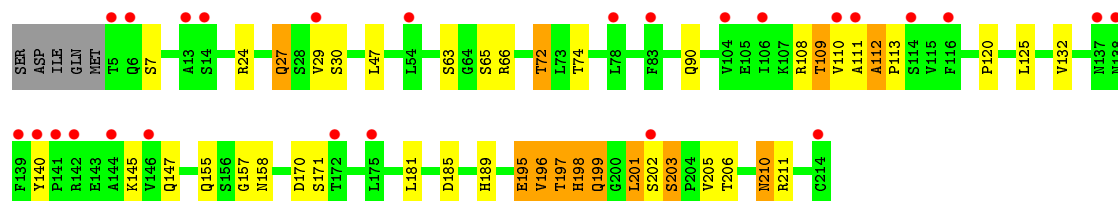
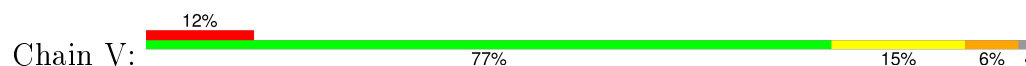


• Molecule 2: FAB LIGHT CHAIN

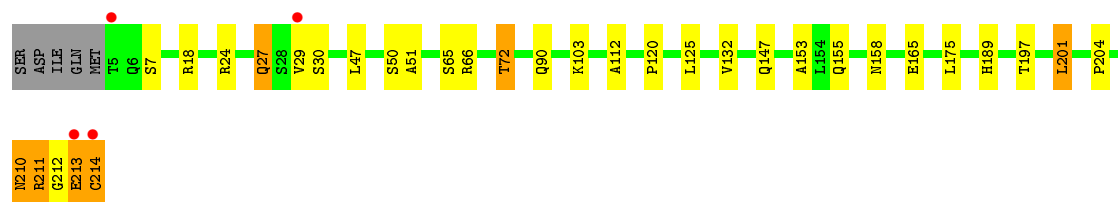
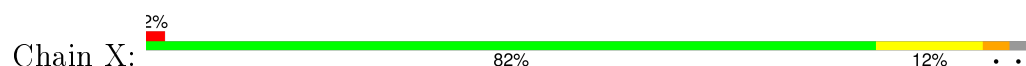
Chain T: 81% 15% ..



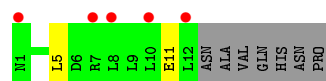
• Molecule 2: FAB LIGHT CHAIN



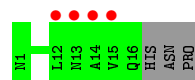
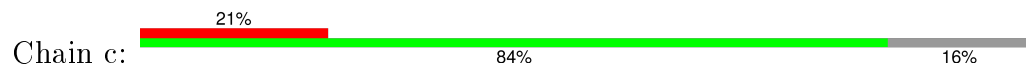
• Molecule 2: FAB LIGHT CHAIN



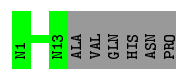
• Molecule 3: PAXILLIN LD2



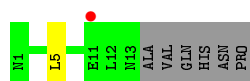
• Molecule 3: PAXILLIN LD2



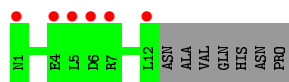
• Molecule 3: PAXILLIN LD2



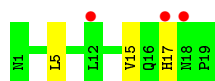
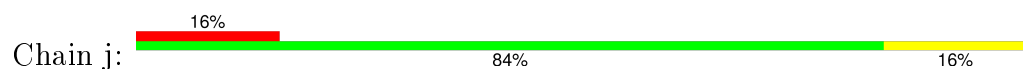
• Molecule 3: PAXILLIN LD2



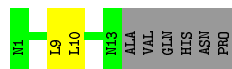
• Molecule 3: PAXILLIN LD2



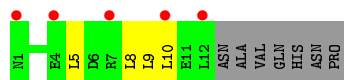
• Molecule 3: PAXILLIN LD2



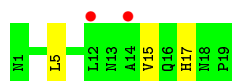
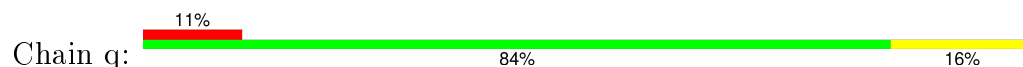
• Molecule 3: PAXILLIN LD2



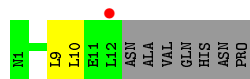
• Molecule 3: PAXILLIN LD2



• Molecule 3: PAXILLIN LD2



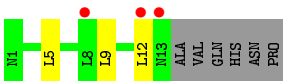
• Molecule 3: PAXILLIN LD2



• Molecule 3: PAXILLIN LD2







● Molecule 3: PAXILLIN LD2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.19Å 111.00Å 143.87Å 94.65° 95.28° 114.53°	Depositor
Resolution (Å)	142.00 – 2.50 100.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.3 (142.00-2.50) 89.9 (100.11-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.228 , 0.245 0.237 , 0.254	Depositor DCC
$R_{free}$ test set	9884 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.0	EDS
Estimated twinning fraction	0.013 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 195832 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	40426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NO3

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	0.47	1/1661 (0.1%)	0.54	0/2265
1	C	0.48	0/1674	0.56	0/2283
1	E	0.48	1/1626 (0.1%)	0.55	1/2216 (0.0%)
1	G	0.46	0/1665	0.55	0/2270
1	H	0.47	0/1675	0.56	0/2283
1	J	0.48	1/1704 (0.1%)	0.57	0/2325
1	M	0.46	0/1684	0.56	0/2295
1	O	0.44	0/1702	0.54	0/2321
1	Q	0.44	0/1659	0.54	0/2264
1	S	0.45	0/1653	0.53	1/2255 (0.0%)
1	U	0.51	1/1659 (0.1%)	0.67	1/2262 (0.0%)
1	W	0.47	0/1665	0.55	0/2270
2	B	0.40	1/1625 (0.1%)	0.59	3/2205 (0.1%)
2	D	0.41	0/1625	0.58	1/2205 (0.0%)
2	F	0.41	0/1600	0.52	0/2173
2	I	0.41	0/1630	0.60	2/2212 (0.1%)
2	K	0.41	0/1625	0.60	2/2205 (0.1%)
2	L	0.39	0/1619	0.57	2/2197 (0.1%)
2	N	0.43	0/1625	0.57	0/2205
2	P	0.41	0/1625	0.56	0/2205
2	R	0.41	0/1633	0.62	2/2215 (0.1%)
2	T	0.43	1/1625 (0.1%)	0.59	2/2205 (0.1%)
2	V	0.48	0/1625	0.65	1/2205 (0.0%)
2	X	0.45	1/1625 (0.1%)	0.57	1/2205 (0.0%)
3	a	1.17	2/98 (2.0%)	1.24	2/131 (1.5%)
3	c	0.40	0/127	0.63	0/171
3	e	0.41	0/106	0.61	0/142
3	g	0.40	0/106	0.61	0/142
3	h	0.48	0/98	0.62	0/131
3	j	0.48	0/154	0.73	0/209
3	m	0.39	0/106	0.66	0/142
3	o	0.41	0/98	0.79	0/131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	q	0.48	0/154	0.70	0/209
3	s	0.50	0/98	0.60	0/131
3	u	0.46	0/106	0.86	0/142
3	w	0.38	0/98	0.61	0/131
All	All	0.45	9/40858 (0.0%)	0.58	21/55558 (0.0%)

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	J	0	1
1	Q	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	11	GLU	CD-OE2	-7.46	1.17	1.25
3	a	11	GLU	CD-OE1	6.15	1.32	1.25
2	X	213	GLU	CG-CD	5.72	1.60	1.51
1	E	105	GLN	C-O	5.60	1.33	1.23
2	B	35	TRP	CD2-CE2	5.11	1.47	1.41
1	J	154	TRP	CD2-CE2	5.11	1.47	1.41
1	U	47	TRP	CD2-CE2	5.07	1.47	1.41
2	T	208	SER	CB-OG	-5.01	1.35	1.42
1	A	154	TRP	CD2-CE2	5.00	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	196	CYS	CA-CB-SG	12.72	136.90	114.00
3	a	11	GLU	CG-CD-OE2	-8.51	101.28	118.30
2	K	211	ARG	NE-CZ-NH1	-8.36	116.12	120.30
3	a	11	GLU	CG-CD-OE1	8.32	134.93	118.30
1	E	105	GLN	N-CA-C	-8.07	89.21	111.00
2	R	211	ARG	NE-CZ-NH1	-8.02	116.29	120.30
2	D	211	ARG	CG-CD-NE	-7.85	95.31	111.80
2	B	211	ARG	N-CA-CB	6.89	123.01	110.60
2	B	211	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	L	27	GLN	CA-CB-CG	6.72	128.18	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	211	ARG	NE-CZ-NH2	6.54	123.57	120.30
2	L	211	ARG	NE-CZ-NH1	-6.28	117.16	120.30
2	R	211	ARG	NE-CZ-NH2	6.14	123.37	120.30
2	T	211	ARG	NE-CZ-NH2	-5.81	117.40	120.30
2	B	211	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	T	211	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	I	211	ARG	CB-CA-C	-5.51	99.38	110.40
1	S	214	LYS	N-CA-C	-5.45	96.30	111.00
2	I	211	ARG	N-CA-C	5.39	125.56	111.00
2	X	213	GLU	OE1-CD-OE2	-5.31	116.93	123.30
2	V	196	VAL	CB-CA-C	-5.29	101.35	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	213	PRO	Peptide
1	Q	214	LYS	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	A	1620	0	1567	10	1
1	C	1633	0	1573	20	0
1	E	1586	0	1537	15	0
1	G	1624	0	1570	10	0
1	H	1634	0	1586	23	0
1	J	1662	0	1600	20	1
1	M	1643	0	1589	33	0
1	O	1660	0	1605	18	0
1	Q	1618	0	1555	9	0
1	S	1612	0	1566	26	0
1	U	1618	0	1565	57	0
1	W	1624	0	1570	16	0
2	B	1593	0	1555	12	0
2	D	1593	0	1555	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1568	0	1531	16	1
2	I	1598	0	1557	13	0
2	K	1593	0	1555	13	0
2	L	1587	0	1551	15	0
2	N	1593	0	1555	27	0
2	P	1593	0	1555	22	0
2	R	1601	0	1564	34	1
2	T	1593	0	1556	16	0
2	V	1593	0	1555	48	0
2	X	1593	0	1555	18	0
3	a	99	0	108	0	0
3	c	128	0	136	0	0
3	e	107	0	114	0	0
3	g	107	0	114	0	0
3	h	99	0	108	0	0
3	j	153	0	156	0	0
3	m	107	0	114	0	0
3	o	99	0	108	0	0
3	q	153	0	156	0	0
3	s	99	0	108	0	0
3	u	107	0	114	0	0
3	w	99	0	108	0	0
4	B	4	0	0	0	0
4	D	4	0	0	0	0
4	F	4	0	0	0	0
4	I	4	0	0	1	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
4	N	4	0	0	0	0
4	P	4	0	0	0	0
4	R	4	0	0	0	0
4	T	4	0	0	0	0
4	V	4	0	0	0	0
4	X	4	0	0	1	0
5	N	4	0	6	0	0
5	Q	4	0	6	0	0
5	W	4	0	6	0	0
6	A	11	0	0	0	0
6	B	5	0	0	1	0
6	C	19	0	0	0	0
6	D	16	0	0	0	0
6	E	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	2	0	0	0	0
6	G	19	0	0	0	0
6	H	29	0	0	3	0
6	I	14	0	0	0	0
6	J	17	0	0	2	0
6	K	13	0	0	0	0
6	L	17	0	0	1	0
6	M	25	0	0	0	0
6	N	31	0	0	2	0
6	O	13	0	0	0	0
6	P	11	0	0	0	0
6	Q	21	0	0	0	0
6	R	20	0	0	1	0
6	S	19	0	0	2	0
6	T	10	0	0	0	0
6	U	10	0	0	0	0
6	V	4	0	0	0	0
6	W	12	0	0	2	0
6	X	12	0	0	0	0
6	a	1	0	0	0	0
6	c	1	0	0	0	0
6	e	1	0	0	0	0
6	g	2	0	0	0	0
6	j	4	0	0	0	0
6	m	1	0	0	0	0
6	o	1	0	0	0	0
6	q	3	0	0	0	0
6	s	1	0	0	0	0
6	u	1	0	0	0	0
6	w	1	0	0	0	0
All	All	40426	0	38989	451	2

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 6.

All (451) 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:U:184:VAL:HG21	1:U:194:TYR:CZ	1.64	1.31
2:V:108:ARG:NH1	2:V:109:THR:O	1.68	1.24
1:M:193:THR:HG22	2:R:77:SER:OG	1.08	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:198:HIS:HB3	2:V:201:LEU:HB3	1.27	1.16
2:V:201:LEU:HD21	2:V:203:SER:O	1.50	1.12
1:M:195:ILE:HD11	2:R:15:VAL:HG11	1.13	1.11
1:M:195:ILE:CD1	2:R:15:VAL:HG11	1.82	1.08
1:M:193:THR:CG2	2:R:77:SER:OG	2.00	1.07
2:V:201:LEU:O	2:V:201:LEU:HD13	1.55	1.06
1:U:184:VAL:HG21	1:U:194:TYR:CE2	1.90	1.06
1:U:188:SER:O	1:U:191:THR:HG23	1.54	1.06
1:U:185:PRO:HG2	1:U:188:SER:HB2	1.34	1.06
1:U:185:PRO:HG2	1:U:188:SER:CB	1.86	1.05
1:M:195:ILE:HD11	2:R:15:VAL:CG1	1.87	1.04
1:U:184:VAL:HG11	1:U:194:TYR:CE1	1.97	0.99
2:F:67:SER:OG	2:V:185:ASP:OD1	1.81	0.98
1:U:184:VAL:CG2	1:U:194:TYR:CZ	2.47	0.97
1:M:193:THR:HG22	2:R:77:SER:HG	1.32	0.94
1:U:184:VAL:CG2	1:U:194:TYR:OH	2.16	0.94
1:M:193:THR:CG2	2:R:16:GLY:HA2	1.98	0.93
2:V:195:GLU:HG3	2:V:195:GLU:O	1.68	0.93
2:V:201:LEU:C	2:V:201:LEU:HD13	1.89	0.92
1:U:185:PRO:CG	1:U:188:SER:HB2	2.01	0.90
1:S:-1:ILE:HG23	1:S:-1:ILE:O	1.75	0.87
2:X:210:ASN:O	2:X:212:GLY:N	2.08	0.87
2:V:111:ALA:O	2:V:112:ALA:HB3	1.76	0.84
1:H:82:MET:HE2	1:H:82(C):LEU:HD11	1.57	0.84
1:U:184:VAL:HG21	1:U:194:TYR:OH	1.77	0.83
1:U:186:SER:O	1:U:189:LEU:HD12	1.78	0.83
2:N:28:SER:C	2:N:30:SER:H	1.82	0.82
2:V:110:VAL:HG13	2:V:140:TYR:O	1.79	0.82
1:U:186:SER:O	1:U:189:LEU:HG	1.79	0.82
1:G:68:THR:HG23	1:G:81:GLN:HB3	1.61	0.81
6:H:324:HOH:O	1:U:18:LEU:HD11	1.81	0.81
1:S:156:SER:H	1:S:197:ASN:HD21	1.26	0.81
2:V:108:ARG:NE	2:V:170:ASP:O	2.14	0.80
2:N:28:SER:O	2:N:30:SER:N	2.14	0.80
1:U:188:SER:O	1:U:191:THR:CG2	2.30	0.80
1:U:186:SER:O	1:U:189:LEU:CD1	2.30	0.80
1:Q:214:LYS:CB	1:Q:216:CYS:O	2.30	0.80
2:V:198:HIS:HB3	2:V:201:LEU:CB	2.09	0.79
2:V:201:LEU:CD1	2:V:201:LEU:O	2.30	0.79
2:V:201:LEU:CD2	2:V:203:SER:O	2.30	0.78
1:S:-1:ILE:O	1:S:-1:ILE:CG2	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:SER:HB3	1:C:73:THR:HG22	1.63	0.78
1:S:82:MET:HE2	1:S:82(C):LEU:HD11	1.65	0.78
1:M:193:THR:HG21	2:R:16:GLY:HA2	1.66	0.77
2:L:155:GLN:HE21	2:L:158:ASN:HD21	1.31	0.77
2:N:155:GLN:HE21	2:N:158:ASN:HD21	1.30	0.77
2:V:111:ALA:O	2:V:112:ALA:CB	2.30	0.77
2:N:210:ASN:OD1	2:P:151:ASP:HB3	1.85	0.77
1:U:186:SER:O	1:U:189:LEU:CG	2.33	0.76
1:G:156:SER:H	1:G:197:ASN:HD21	1.32	0.76
2:V:113:PRO:CG	2:V:198:HIS:ND1	2.49	0.76
1:W:156:SER:H	1:W:197:ASN:HD21	1.32	0.76
1:M:195:ILE:CD1	2:R:15:VAL:CG1	2.56	0.76
1:A:82:MET:HE2	1:A:82(C):LEU:HD11	1.66	0.76
2:V:63:SER:OG	2:V:74:THR:HG22	1.86	0.75
1:E:156:SER:H	1:E:197:ASN:HD21	1.32	0.75
1:H:121:VAL:HG21	1:H:207:VAL:HG11	1.68	0.75
1:J:156:SER:H	1:J:197:ASN:HD21	1.32	0.75
2:D:155:GLN:HE21	2:D:158:ASN:HD21	1.32	0.75
1:Q:82:MET:HE2	1:Q:82(C):LEU:HD11	1.68	0.74
1:Q:156:SER:H	1:Q:197:ASN:HD21	1.34	0.74
1:J:82:MET:HE2	1:J:82(C):LEU:HD11	1.69	0.73
1:H:156:SER:H	1:H:197:ASN:HD21	1.37	0.73
1:J:18:LEU:HD11	6:J:315:HOH:O	1.87	0.73
2:L:27:GLN:C	2:L:27:GLN:HE21	1.91	0.73
1:W:82:MET:HE2	1:W:82(C):LEU:HD11	1.70	0.73
1:U:156:SER:H	1:U:197:ASN:HD21	1.35	0.72
1:O:156:SER:H	1:O:197:ASN:HD21	1.37	0.72
2:V:205:VAL:CG1	2:V:206:THR:N	2.52	0.71
2:N:191:VAL:HG11	2:P:191:VAL:HG11	1.73	0.71
1:W:193:THR:HG22	6:W:402:HOH:O	1.88	0.71
1:E:74:SER:HB2	1:S:158:ALA:O	1.89	0.71
2:B:197:THR:HG23	6:B:401:HOH:O	1.90	0.71
2:R:197:THR:HG23	6:R:403:HOH:O	1.90	0.71
1:G:82:MET:HE2	1:G:82(C):LEU:HD11	1.71	0.71
1:C:156:SER:H	1:C:197:ASN:HD21	1.37	0.70
2:V:195:GLU:CG	2:V:195:GLU:O	2.40	0.70
2:D:147:GLN:HG2	2:D:154:LEU:HD22	1.75	0.69
1:M:156:SER:H	1:M:197:ASN:HD21	1.38	0.69
1:M:121:VAL:HG21	1:M:207:VAL:HG11	1.74	0.69
2:X:155:GLN:HE21	2:X:158:ASN:HD21	1.39	0.69
1:U:82:MET:HE2	1:U:82(C):LEU:HD11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:197:THR:OG1	2:V:198:HIS:N	2.21	0.68
1:E:82:MET:HE2	1:E:82(C):LEU:HD11	1.75	0.68
2:V:63:SER:OG	2:V:74:THR:CG2	2.42	0.67
2:D:211:ARG:NH1	2:D:211:ARG:HG2	2.10	0.67
2:I:153:ALA:HB2	2:R:18:ARG:HD3	1.76	0.66
1:H:121:VAL:HG21	1:H:207:VAL:CG1	2.26	0.66
1:H:75:LYS:NZ	1:J:73:THR:HB	2.10	0.66
1:S:214:LYS:NZ	2:T:122:ASP:OD2	2.29	0.66
2:P:213:GLU:HG2	2:P:214:CYS:N	2.09	0.65
2:B:155:GLN:HE21	2:B:158:ASN:HD21	1.42	0.65
1:U:184:VAL:CB	1:U:194:TYR:OH	2.44	0.65
1:U:185:PRO:HD2	1:U:194:TYR:OH	1.96	0.65
2:V:108:ARG:HD2	2:V:171:SER:HB2	1.79	0.65
1:M:129:LYS:H	1:M:130:SER:C	2.00	0.65
2:R:155:GLN:HE21	2:R:158:ASN:HD21	1.44	0.65
1:S:2:VAL:HG12	6:S:319:HOH:O	1.96	0.65
1:U:182:VAL:O	1:U:182:VAL:HG13	1.97	0.65
1:H:121:VAL:CG2	1:H:207:VAL:HG11	2.28	0.64
2:P:155:GLN:HE21	2:P:158:ASN:HD21	1.45	0.64
1:O:31:TYR:CE1	1:S:206:LYS:NZ	2.65	0.64
1:U:184:VAL:HB	1:U:194:TYR:OH	1.97	0.64
1:S:135:THR:N	6:S:314:HOH:O	2.31	0.63
2:T:210:ASN:HD22	2:T:210:ASN:N	1.96	0.63
2:V:205:VAL:HG12	2:V:206:THR:N	2.12	0.63
1:J:18:LEU:CD1	6:J:315:HOH:O	2.47	0.61
1:U:184:VAL:HB	1:U:185:PRO:HD2	1.82	0.61
2:P:152:ASN:C	2:P:152:ASN:OD1	2.39	0.61
2:X:210:ASN:N	2:X:210:ASN:HD22	1.98	0.61
1:O:11:LEU:HD22	1:O:12:VAL:N	2.16	0.61
2:K:210:ASN:N	2:K:210:ASN:HD22	1.99	0.61
2:F:210:ASN:N	2:F:210:ASN:HD22	1.99	0.61
2:N:152:ASN:OD1	2:N:152:ASN:C	2.40	0.60
2:V:197:THR:O	2:V:198:HIS:HB2	1.99	0.60
1:U:185:PRO:HG2	1:U:188:SER:HB3	1.79	0.60
1:M:121:VAL:CG2	1:M:207:VAL:HG11	2.32	0.60
2:D:153:ALA:HB2	2:N:18:ARG:HD3	1.83	0.60
1:M:121:VAL:HG21	1:M:207:VAL:CG1	2.31	0.60
2:B:210:ASN:HD22	2:B:210:ASN:N	1.98	0.60
2:B:153:ALA:HB2	2:T:18:ARG:HD3	1.83	0.60
2:N:210:ASN:HD22	2:N:210:ASN:N	2.00	0.60
2:T:29:VAL:HG13	2:T:66:ARG:HH21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:181:VAL:HG23	1:U:181:VAL:O	2.02	0.60
1:C:2:VAL:HG11	1:C:102:TYR:CE2	2.37	0.60
2:K:29:VAL:HG13	2:K:66:ARG:HH21	1.67	0.60
2:P:29:VAL:HG13	2:P:66:ARG:HH21	1.67	0.60
2:D:210:ASN:N	2:D:210:ASN:HD22	1.99	0.60
1:U:185:PRO:O	1:U:188:SER:N	2.30	0.59
2:F:67:SER:CB	2:V:185:ASP:OD1	2.49	0.59
1:U:184:VAL:CB	1:U:185:PRO:HD2	2.32	0.59
2:V:201:LEU:C	2:V:201:LEU:CD1	2.63	0.59
2:B:18:ARG:HD3	2:T:153:ALA:HB2	1.85	0.59
6:H:324:HOH:O	1:U:18:LEU:CD1	2.46	0.59
2:B:29:VAL:HG13	2:B:66:ARG:HH21	1.68	0.59
2:B:187:GLU:OE2	2:B:211:ARG:NH1	2.36	0.58
2:V:210:ASN:N	2:V:210:ASN:HD22	2.02	0.58
1:S:178:LEU:HD12	1:S:178:LEU:C	2.24	0.58
2:L:29:VAL:HG13	2:L:66:ARG:HH21	1.68	0.58
2:N:28:SER:C	2:N:30:SER:N	2.44	0.58
2:V:113:PRO:HG3	2:V:198:HIS:ND1	2.18	0.58
2:X:65:SER:HB3	2:X:72:THR:HG22	1.86	0.58
1:A:156:SER:H	1:A:197:ASN:HD21	1.51	0.58
1:G:2:VAL:HG11	1:G:102:TYR:CZ	2.39	0.57
2:N:151:ASP:HB3	2:P:210:ASN:OD1	2.04	0.57
1:H:129:LYS:O	1:H:129:LYS:HG2	2.05	0.57
2:V:145:LYS:HE2	2:V:197:THR:HG21	1.87	0.57
1:S:2:VAL:HG11	1:S:102:TYR:CE2	2.38	0.57
2:F:29:VAL:HG13	2:F:66:ARG:HH21	1.69	0.57
1:O:82:MET:HE2	1:O:82(C):LEU:HD11	1.87	0.57
2:V:113:PRO:HD3	2:V:198:HIS:CE1	2.39	0.57
2:T:112:ALA:HB1	2:T:201:LEU:CD1	2.34	0.57
1:U:184:VAL:CB	1:U:194:TYR:CZ	2.87	0.56
2:R:210:ASN:N	2:R:210:ASN:HD22	2.02	0.56
1:M:82:MET:HE3	1:M:90:TYR:CE2	2.40	0.56
2:I:155:GLN:HE21	2:I:158:ASN:HD21	1.52	0.56
2:L:210:ASN:HD22	2:L:210:ASN:N	2.03	0.56
1:E:2:VAL:HG11	1:E:102:TYR:CE2	2.40	0.56
2:I:210:ASN:N	2:I:210:ASN:HD22	2.04	0.56
2:R:198:HIS:CD2	2:R:200:GLY:H	2.24	0.56
2:X:29:VAL:HG13	2:X:66:ARG:HH21	1.70	0.56
2:N:31:SER:HA	2:N:71:PHE:CZ	2.40	0.56
1:U:184:VAL:HG23	1:U:185:PRO:HD2	1.88	0.56
1:C:2:VAL:HG11	1:C:102:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:SER:HB3	2:D:72:THR:HG22	1.88	0.56
2:V:113:PRO:HG3	2:V:198:HIS:CE1	2.41	0.56
1:S:2:VAL:HG11	1:S:102:TYR:CZ	2.40	0.56
1:M:210:LYS:O	1:M:210:LYS:HG3	2.06	0.56
2:B:65:SER:HB3	2:B:72:THR:HG22	1.88	0.56
2:I:29:VAL:HG13	2:I:66:ARG:HH21	1.71	0.55
1:O:73:THR:HG22	1:S:156:SER:CB	2.36	0.55
2:P:65:SER:HB3	2:P:72:THR:HG22	1.89	0.55
1:A:178:LEU:HD12	1:A:178:LEU:C	2.27	0.55
2:R:29:VAL:HG13	2:R:66:ARG:HH21	1.71	0.55
2:T:65:SER:HB3	2:T:72:THR:HG22	1.88	0.55
2:K:155:GLN:HE21	2:K:158:ASN:HD21	1.54	0.55
1:W:2:VAL:HG11	1:W:102:TYR:CZ	2.42	0.55
1:U:66:ARG:NH2	1:U:86:ASP:OD2	2.40	0.55
2:V:196:VAL:HG12	2:V:197:THR:O	2.06	0.55
2:D:29:VAL:HG13	2:D:66:ARG:HH21	1.71	0.55
1:E:2:VAL:HG11	1:E:102:TYR:CZ	2.42	0.55
2:L:65:SER:HB3	2:L:72:THR:HG22	1.89	0.55
2:D:199:GLN:HA	2:N:199:GLN:HG3	1.89	0.55
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.40	0.55
1:O:66:ARG:NH2	1:O:86:ASP:OD2	2.40	0.54
1:W:66:ARG:NH2	1:W:86:ASP:OD2	2.41	0.54
1:Q:66:ARG:NH2	1:Q:86:ASP:OD2	2.40	0.54
1:H:178:LEU:C	1:H:178:LEU:HD12	2.27	0.54
1:C:2:VAL:CG1	1:C:102:TYR:CZ	2.90	0.54
2:K:65:SER:HB3	2:K:72:THR:HG22	1.88	0.54
1:H:18:LEU:HD13	1:J:56:TYR:CE1	2.42	0.54
2:V:65:SER:HB3	2:V:72:THR:HG22	1.89	0.54
2:I:65:SER:HB3	2:I:72:THR:HG22	1.90	0.54
1:A:2:VAL:HG11	1:A:102:TYR:CE2	2.42	0.54
1:J:66:ARG:NH2	1:J:86:ASP:OD2	2.40	0.54
2:F:65:SER:HB3	2:F:72:THR:HG22	1.89	0.54
1:A:66:ARG:NH2	1:A:86:ASP:OD2	2.40	0.54
2:N:106:ILE:HD12	6:N:429:HOH:O	2.07	0.54
1:S:66:ARG:NH2	1:S:86:ASP:OD2	2.41	0.54
2:P:210:ASN:HD22	2:P:210:ASN:N	2.05	0.54
2:K:18:ARG:HD3	2:P:153:ALA:HB2	1.90	0.54
1:G:66:ARG:NH2	1:G:86:ASP:OD2	2.41	0.54
1:C:66:ARG:NH2	1:C:86:ASP:OD2	2.41	0.54
1:M:66:ARG:NH2	1:M:86:ASP:OD2	2.41	0.54
2:L:27:GLN:HE21	2:L:27:GLN:CA	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:VAL:HG11	1:A:102:TYR:CZ	2.44	0.53
1:M:178:LEU:C	1:M:178:LEU:HD12	2.28	0.53
1:U:2:VAL:HG11	1:U:102:TYR:CZ	2.44	0.53
1:Q:178:LEU:HD12	1:Q:178:LEU:C	2.29	0.53
2:L:112:ALA:HB1	2:L:201:LEU:CD1	2.38	0.53
2:F:155:GLN:HE21	2:F:158:ASN:HD21	1.55	0.53
1:U:184:VAL:CG1	1:U:194:TYR:CE1	2.83	0.53
1:S:2:VAL:CG1	1:S:102:TYR:CZ	2.91	0.53
2:L:27:GLN:HB3	2:L:90:GLN:HG3	1.90	0.53
1:E:66:ARG:NH2	1:E:86:ASP:OD2	2.41	0.53
1:J:183:THR:HG21	2:K:137:ASN:ND2	2.24	0.53
1:O:31:TYR:CZ	1:S:206:LYS:NZ	2.77	0.53
1:M:129:LYS:N	1:M:130:SER:C	2.62	0.53
1:S:2:VAL:HG13	1:S:102:TYR:CE1	2.44	0.53
1:J:166:PHE:CE1	2:K:164:THR:HG23	2.44	0.53
2:K:112:ALA:HB1	2:K:201:LEU:CD1	2.38	0.53
1:E:2:VAL:CG1	1:E:102:TYR:CZ	2.92	0.53
2:X:112:ALA:HB1	2:X:201:LEU:CD1	2.40	0.52
2:P:189:HIS:O	2:P:211:ARG:NH1	2.42	0.52
2:L:18:ARG:HD3	2:X:153:ALA:HB2	1.89	0.52
1:G:2:VAL:CG1	1:G:102:TYR:CZ	2.92	0.52
2:N:65:SER:HB3	2:N:72:THR:HG22	1.90	0.52
1:H:75:LYS:HZ3	1:J:73:THR:HB	1.75	0.52
2:N:112:ALA:HB1	2:N:201:LEU:CD1	2.40	0.52
2:N:189:HIS:O	2:N:211:ARG:NH1	2.43	0.52
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.91	0.52
1:C:2:VAL:HG13	1:C:102:TYR:CE1	2.45	0.52
2:X:189:HIS:O	2:X:211:ARG:NH1	2.42	0.52
2:I:189:HIS:O	2:I:211:ARG:NH1	2.42	0.52
1:A:2:VAL:CG1	1:A:102:TYR:CZ	2.93	0.52
1:G:2:VAL:HG11	1:G:102:TYR:CE2	2.45	0.52
1:H:129:LYS:CG	1:H:129:LYS:O	2.57	0.51
2:V:189:HIS:O	2:V:211:ARG:NH1	2.42	0.51
1:E:2:VAL:HG13	1:E:102:TYR:CE1	2.45	0.51
1:U:184:VAL:CG2	1:U:185:PRO:HD2	2.41	0.51
1:M:198:VAL:HB	1:M:207:VAL:HG12	1.93	0.51
1:G:2:VAL:HG13	1:G:102:TYR:CE1	2.46	0.51
2:R:197:THR:HG22	2:R:204:PRO:HB3	1.93	0.51
1:A:2:VAL:HG13	1:A:102:TYR:CE1	2.45	0.51
2:P:213:GLU:CG	2:P:214:CYS:N	2.74	0.51
2:K:197:THR:HG22	2:K:204:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:LEU:HD12	1:E:178:LEU:C	2.31	0.51
1:J:2:VAL:HG11	1:J:102:TYR:CZ	2.45	0.51
1:Q:143:LYS:HE2	1:Q:171:GLN:HE22	1.76	0.51
1:H:73:THR:HB	1:U:75:LYS:NZ	2.25	0.51
2:D:147:GLN:HG2	2:D:154:LEU:CD2	2.39	0.51
2:T:155:GLN:HE21	2:T:158:ASN:HD21	1.58	0.51
2:R:4:MET:O	2:R:5:THR:OG1	2.26	0.51
1:O:73:THR:HG22	1:S:156:SER:HB2	1.91	0.51
2:V:155:GLN:HE21	2:V:158:ASN:HD21	1.59	0.51
1:S:214:LYS:CG	1:S:215:SER:N	2.74	0.50
2:I:197:THR:HG22	2:I:204:PRO:HB3	1.93	0.50
1:U:188:SER:C	1:U:191:THR:HG23	2.28	0.50
1:C:216:CYS:O	1:C:217:ASP:CB	2.59	0.50
2:P:112:ALA:HB1	2:P:201:LEU:CD1	2.40	0.50
1:C:82:MET:CE	1:C:82(C):LEU:HD11	2.41	0.50
1:O:143:LYS:HE2	1:O:171:GLN:HE22	1.76	0.50
2:D:175:LEU:HD23	2:D:176:SER:N	2.26	0.50
2:D:189:HIS:O	2:D:211:ARG:NH1	2.43	0.50
2:N:151:ASP:O	2:N:152:ASN:CG	2.50	0.50
1:U:178:LEU:HD12	1:U:178:LEU:C	2.32	0.50
2:N:29:VAL:HG23	2:N:66:ARG:HH21	1.76	0.50
1:C:178:LEU:C	1:C:178:LEU:HD12	2.32	0.50
1:H:56:TYR:CE1	1:U:18:LEU:HD13	2.46	0.50
1:U:184:VAL:HG11	1:U:194:TYR:CZ	2.45	0.50
1:H:198:VAL:HB	1:H:207:VAL:HG12	1.94	0.50
1:M:82:MET:CE	1:M:90:TYR:CZ	2.95	0.49
2:X:212:GLY:C	2:X:214:CYS:H	2.15	0.49
1:J:192:GLN:NE2	1:J:193:THR:H	2.10	0.49
2:V:108:ARG:HG2	2:V:109:THR:N	2.26	0.49
1:C:30:SER:HB3	1:C:73:THR:CG2	2.39	0.49
1:E:56:TYR:CE1	1:W:18:LEU:HD13	2.47	0.49
2:L:197:THR:HG22	2:L:204:PRO:HB3	1.93	0.49
2:F:197:THR:HG22	2:F:204:PRO:HB3	1.95	0.49
2:F:24:ARG:HD3	2:V:157:GLY:HA2	1.95	0.49
2:X:197:THR:HG22	2:X:204:PRO:HB3	1.94	0.49
2:R:112:ALA:HB1	2:R:201:LEU:CD1	2.43	0.49
2:X:24:ARG:NH2	4:X:301:NO3:O2	2.43	0.49
2:P:197:THR:HG22	2:P:204:PRO:HB3	1.95	0.49
1:H:18:LEU:HD13	1:J:56:TYR:CD1	2.47	0.49
2:N:197:THR:HG22	2:N:204:PRO:HB3	1.95	0.49
1:M:123:PRO:HD3	1:M:209:LYS:NZ	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:143:LYS:HE2	1:J:171:GLN:HE22	1.77	0.48
1:S:143:LYS:HE2	1:S:171:GLN:HE22	1.78	0.48
1:C:143:LYS:HE2	1:C:171:GLN:HE22	1.79	0.48
2:F:112:ALA:HB1	2:F:201:LEU:CD1	2.44	0.48
2:B:112:ALA:HB1	2:B:201:LEU:CD1	2.43	0.48
2:V:113:PRO:CD	2:V:198:HIS:ND1	2.77	0.48
1:U:2:VAL:CG1	1:U:102:TYR:CZ	2.96	0.48
2:V:145:LYS:HB3	2:V:197:THR:HG23	1.95	0.48
1:W:2:VAL:CG1	1:W:102:TYR:CZ	2.96	0.48
1:E:73:THR:HB	1:W:75:LYS:NZ	2.27	0.48
1:U:193:THR:O	1:U:193:THR:OG1	2.30	0.48
2:D:175:LEU:C	2:D:175:LEU:HD23	2.35	0.48
2:T:197:THR:HG22	2:T:204:PRO:HB3	1.96	0.48
1:W:143:LYS:HE2	1:W:171:GLN:HE22	1.79	0.48
2:L:189:HIS:O	2:L:211:ARG:NH2	2.46	0.47
1:G:143:LYS:HE2	1:G:171:GLN:HE22	1.78	0.47
1:J:178:LEU:HD12	1:J:178:LEU:C	2.34	0.47
2:V:113:PRO:CD	2:V:198:HIS:CE1	2.97	0.47
2:V:113:PRO:HG2	2:V:198:HIS:ND1	2.28	0.47
1:E:143:LYS:HE2	1:E:171:GLN:HE22	1.80	0.47
1:C:82:MET:HE2	1:C:82(C):LEU:HD11	1.96	0.47
1:M:193:THR:N	2:R:77:SER:OG	2.44	0.47
2:I:18:ARG:HD3	2:R:153:ALA:HB2	1.97	0.47
1:U:2:VAL:HG11	1:U:102:TYR:CE2	2.50	0.47
1:O:73:THR:CG2	1:S:156:SER:HB3	2.44	0.47
2:I:37:GLN:HB2	2:I:47:LEU:HD21	1.95	0.47
1:U:186:SER:HA	1:U:189:LEU:HD11	1.97	0.47
1:U:2:VAL:HG13	1:U:102:TYR:CE1	2.49	0.47
1:W:2:VAL:HG13	1:W:102:TYR:CE1	2.50	0.47
2:T:103:LYS:NZ	2:T:165:GLU:OE1	2.42	0.47
1:G:147:PRO:O	1:G:200:HIS:HE1	1.98	0.47
1:C:216:CYS:O	1:C:217:ASP:HB2	2.16	0.46
2:V:108:ARG:HG2	2:V:109:THR:H	1.80	0.46
2:P:120:PRO:HD3	2:P:132:VAL:HG22	1.97	0.46
2:V:113:PRO:CG	2:V:198:HIS:CE1	2.98	0.46
2:D:147:GLN:HE22	2:N:12:SER:HB2	1.81	0.46
1:M:143:LYS:HE2	1:M:171:GLN:HE22	1.81	0.46
2:V:199:GLN:HB3	2:V:199:GLN:HE21	1.36	0.46
1:W:193:THR:HG23	6:W:403:HOH:O	2.15	0.46
1:H:56:TYR:CD1	1:U:18:LEU:HD13	2.50	0.46
2:P:103:LYS:NZ	2:P:165:GLU:OE1	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:82:MET:HE1	1:M:90:TYR:CZ	2.51	0.46
1:H:147:PRO:O	1:H:200:HIS:HE1	1.99	0.46
2:V:29:VAL:HG13	2:V:66:ARG:HH21	1.80	0.46
1:O:73:THR:CG2	1:S:156:SER:CB	2.93	0.46
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.98	0.46
2:P:150:VAL:HG12	2:P:155:GLN:OE1	2.15	0.46
1:U:184:VAL:HG23	1:U:185:PRO:CD	2.46	0.46
1:W:147:PRO:O	1:W:200:HIS:HE1	1.99	0.46
2:K:120:PRO:HD3	2:K:132:VAL:HG22	1.97	0.45
1:U:147:PRO:O	1:U:200:HIS:HE1	1.99	0.45
1:M:147:PRO:O	1:M:200:HIS:HE1	1.98	0.45
2:L:153:ALA:HB2	2:X:18:ARG:HD3	1.96	0.45
2:N:29:VAL:HG13	2:N:29:VAL:O	2.15	0.45
2:K:12:SER:HB2	2:P:147:GLN:HE22	1.82	0.45
1:A:147:PRO:O	1:A:200:HIS:HE1	1.99	0.45
1:H:198:VAL:HB	1:H:207:VAL:CG1	2.46	0.45
1:J:192:GLN:NE2	1:J:193:THR:N	2.65	0.45
1:E:147:PRO:O	1:E:200:HIS:HE1	2.00	0.45
1:H:28:ASN:ND2	6:H:305:HOH:O	2.39	0.45
1:J:147:PRO:O	1:J:200:HIS:HE1	1.99	0.45
1:Q:45:LEU:HD22	2:R:87:TYR:CD2	2.51	0.45
2:V:205:VAL:HG13	2:V:206:THR:N	2.30	0.45
1:C:147:PRO:O	1:C:200:HIS:HE1	2.00	0.45
2:R:4:MET:HG3	2:R:5:THR:HG23	1.99	0.45
1:O:82:MET:CE	1:O:82(C):LEU:HD11	2.46	0.45
2:D:112:ALA:HB1	2:D:201:LEU:CD1	2.46	0.45
1:E:18:LEU:HD13	1:O:56:TYR:CE1	2.51	0.45
2:I:163:VAL:HG22	2:I:175:LEU:HD12	1.97	0.45
2:P:151:ASP:O	2:P:152:ASN:CG	2.55	0.44
1:O:147:PRO:O	1:O:200:HIS:HE1	2.00	0.44
1:J:2:VAL:CG1	1:J:102:TYR:CZ	3.00	0.44
1:W:2:VAL:HG11	1:W:102:TYR:CE2	2.51	0.44
1:S:156:SER:N	1:S:197:ASN:HD21	2.03	0.44
1:J:2:VAL:HG13	1:J:102:TYR:CE1	2.52	0.44
2:T:119:PRO:HB3	2:T:209:PHE:CE2	2.51	0.44
1:M:82:MET:HE3	1:M:90:TYR:CZ	2.53	0.44
1:Q:147:PRO:O	1:Q:200:HIS:HE1	2.00	0.44
1:O:178:LEU:HD12	1:O:178:LEU:C	2.37	0.44
1:S:147:PRO:O	1:S:200:HIS:HE1	2.00	0.44
1:U:182:VAL:O	1:U:182:VAL:CG1	2.65	0.44
2:T:186:TYR:CE1	2:T:192:TYR:CE2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:LEU:CD2	2:F:82:ASP:HB2	2.48	0.44
2:D:18:ARG:HD3	2:N:153:ALA:HB2	1.98	0.44
1:M:191:THR:O	2:R:77:SER:CB	2.67	0.43
2:V:27:GLN:HB2	2:V:90:GLN:HG3	2.00	0.43
2:F:186:TYR:CE1	2:F:192:TYR:CE2	3.06	0.43
1:U:184:VAL:CB	1:U:185:PRO:CD	2.96	0.43
1:S:214:LYS:HE2	1:S:214:LYS:HB2	1.72	0.43
1:C:67:PHE:CZ	1:C:82:MET:HE3	2.54	0.43
1:Q:2:VAL:HG13	1:Q:27:PHE:CD1	2.53	0.43
2:X:27:GLN:HB2	2:X:90:GLN:HG3	2.01	0.43
2:X:120:PRO:HD3	2:X:132:VAL:HG22	2.01	0.43
2:X:103:LYS:NZ	2:X:165:GLU:OE1	2.41	0.43
2:N:27:GLN:HB2	2:N:90:GLN:HG3	2.00	0.43
2:D:155:GLN:NE2	2:D:158:ASN:HD21	2.09	0.43
1:C:82:MET:HB3	1:C:82(C):LEU:HD11	1.99	0.43
2:I:27:GLN:HB2	2:I:90:GLN:HG3	2.01	0.43
2:N:9:SER:HB3	6:N:430:HOH:O	2.17	0.43
2:P:27:GLN:HB2	2:P:90:GLN:HG3	2.01	0.43
2:V:108:ARG:CD	2:V:170:ASP:O	2.67	0.43
1:A:2:VAL:HG23	1:A:27:PHE:CD1	2.54	0.43
2:D:27:GLN:HB2	2:D:90:GLN:HG3	2.00	0.43
1:U:188:SER:C	1:U:191:THR:CG2	2.87	0.43
2:V:120:PRO:HD3	2:V:132:VAL:HG22	2.00	0.43
1:U:143:LYS:HE2	1:U:171:GLN:HE22	1.84	0.43
2:K:27:GLN:HB2	2:K:90:GLN:HG3	2.01	0.43
2:R:175:LEU:HD23	2:R:176:SER:N	2.34	0.43
2:R:27:GLN:HB2	2:R:90:GLN:HG3	2.00	0.43
2:B:27:GLN:HB2	2:B:90:GLN:HG3	2.01	0.42
2:L:120:PRO:HD3	2:L:132:VAL:HG22	2.01	0.42
2:F:120:PRO:HD3	2:F:132:VAL:HG22	2.02	0.42
2:R:209:PHE:C	2:R:210:ASN:HD22	2.23	0.42
1:C:166:PHE:CE2	2:D:176:SER:HB3	2.54	0.42
1:E:56:TYR:CD1	1:W:18:LEU:HD13	2.54	0.42
2:R:175:LEU:HD23	2:R:175:LEU:C	2.39	0.42
1:M:166:PHE:CE1	2:N:164:THR:HG23	2.54	0.42
1:H:73:THR:HB	1:U:75:LYS:HZ3	1.84	0.42
1:U:185:PRO:O	1:U:186:SER:C	2.57	0.42
2:I:120:PRO:HD3	2:I:132:VAL:HG22	2.00	0.42
2:I:24:ARG:NH2	4:I:301:NO3:O1	2.53	0.42
2:D:11:LEU:HD12	2:N:147:GLN:CD	2.40	0.42
1:H:131:THR:O	1:H:133:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:GLN:HB2	2:F:90:GLN:HG3	2.01	0.42
1:O:2:VAL:HG13	1:O:27:PHE:CD1	2.54	0.42
1:U:135:THR:CG2	1:U:183:THR:HB	2.50	0.42
1:C:43:LYS:HE3	2:D:7:SER:OG	2.20	0.42
2:R:45:LYS:CE	2:R:45:LYS:HA	2.49	0.41
2:F:146:VAL:CG1	2:F:147:GLN:N	2.82	0.41
1:U:185:PRO:O	1:U:185:PRO:HG2	2.20	0.41
2:P:150:VAL:CG1	2:P:155:GLN:OE1	2.68	0.41
2:R:120:PRO:HD3	2:R:132:VAL:HG22	2.02	0.41
2:P:150:VAL:HG12	2:P:155:GLN:CD	2.41	0.41
2:T:27:GLN:HB2	2:T:90:GLN:HG3	2.01	0.41
1:M:2:VAL:HG13	1:M:27:PHE:CD1	2.55	0.41
1:M:190:GLY:O	2:R:61:ARG:HB3	2.21	0.41
1:U:188:SER:HA	1:U:191:THR:CG2	2.49	0.41
1:M:191:THR:O	2:R:77:SER:HB3	2.20	0.41
2:F:78:LEU:HD13	2:F:83:PHE:CZ	2.56	0.41
1:C:28:ASN:HD22	1:C:29:VAL:N	2.18	0.41
2:T:175:LEU:HD23	2:T:176:SER:N	2.36	0.41
1:O:18:LEU:HD13	1:W:56:TYR:CE1	2.55	0.41
1:W:82:MET:HB3	1:W:82(C):LEU:HD11	2.03	0.41
1:H:28:ASN:HD22	1:H:29:VAL:N	2.18	0.41
2:L:32:ALA:HA	6:L:417:HOH:O	2.19	0.41
2:N:155:GLN:HE21	2:N:158:ASN:ND2	2.07	0.41
1:O:216:CYS:O	1:O:217:ASP:C	2.57	0.41
1:M:195:ILE:HD12	2:R:15:VAL:CG1	2.49	0.41
1:U:4:LEU:HD21	1:U:27:PHE:CZ	2.56	0.41
2:T:120:PRO:HD3	2:T:132:VAL:HG22	2.02	0.41
2:K:210:ASN:N	2:K:210:ASN:ND2	2.68	0.40
1:J:2:VAL:HG11	1:J:102:TYR:CE2	2.56	0.40
1:S:45:LEU:HD22	2:T:87:TYR:CD2	2.56	0.40
2:L:155:GLN:NE2	2:L:158:ASN:HD21	2.09	0.40
2:X:50:SER:O	2:X:51:ALA:HB3	2.21	0.40
2:F:210:ASN:N	2:F:210:ASN:ND2	2.68	0.40
2:D:210:ASN:N	2:D:210:ASN:ND2	2.67	0.40
2:X:175:LEU:HD23	2:X:175:LEU:C	2.42	0.40
2:X:210:ASN:N	2:X:210:ASN:ND2	2.68	0.40
2:R:112:ALA:HB1	2:R:201:LEU:HD13	2.03	0.40
2:R:44:PRO:O	2:R:45:LYS:HE2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:18:ARG:NH2	2:R:213:GLU:OE2[1_454]	2.07	0.13
1:A:5:VAL:CG1	1:J:191:THR:CG2[1_554]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/229 (93%)	213 (100%)	0	0	100	100
1	C	215/229 (94%)	215 (100%)	0	0	100	100
1	E	206/229 (90%)	206 (100%)	0	0	100	100
1	G	214/229 (93%)	211 (99%)	2 (1%)	1 (0%)	34	55
1	H	215/229 (94%)	213 (99%)	2 (1%)	0	100	100
1	J	222/229 (97%)	220 (99%)	1 (0%)	1 (0%)	34	55
1	M	216/229 (94%)	215 (100%)	0	1 (0%)	34	55
1	O	221/229 (96%)	218 (99%)	2 (1%)	1 (0%)	34	55
1	Q	213/229 (93%)	212 (100%)	1 (0%)	0	100	100
1	S	211/229 (92%)	210 (100%)	1 (0%)	0	100	100
1	U	213/229 (93%)	211 (99%)	1 (0%)	1 (0%)	34	55
1	W	214/229 (93%)	212 (99%)	1 (0%)	1 (0%)	34	55
2	B	208/215 (97%)	202 (97%)	6 (3%)	0	100	100
2	D	208/215 (97%)	202 (97%)	6 (3%)	0	100	100
2	F	205/215 (95%)	199 (97%)	6 (3%)	0	100	100
2	I	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
2	K	208/215 (97%)	202 (97%)	6 (3%)	0	100	100
2	L	207/215 (96%)	200 (97%)	7 (3%)	0	100	100
2	N	208/215 (97%)	201 (97%)	6 (3%)	1 (0%)	34	55
2	P	208/215 (97%)	202 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
2	T	208/215 (97%)	201 (97%)	7 (3%)	0	100	100
2	V	208/215 (97%)	199 (96%)	7 (3%)	2 (1%)	19	34
2	X	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	34	55
3	a	10/19 (53%)	10 (100%)	0	0	100	100
3	c	14/19 (74%)	14 (100%)	0	0	100	100
3	e	11/19 (58%)	11 (100%)	0	0	100	100
3	g	11/19 (58%)	11 (100%)	0	0	100	100
3	h	10/19 (53%)	10 (100%)	0	0	100	100
3	j	17/19 (90%)	15 (88%)	2 (12%)	0	100	100
3	m	11/19 (58%)	11 (100%)	0	0	100	100
3	o	10/19 (53%)	10 (100%)	0	0	100	100
3	q	17/19 (90%)	15 (88%)	2 (12%)	0	100	100
3	s	10/19 (53%)	10 (100%)	0	0	100	100
3	u	11/19 (58%)	11 (100%)	0	0	100	100
3	w	10/19 (53%)	10 (100%)	0	0	100	100
All	All	5209/5556 (94%)	5108 (98%)	91 (2%)	10 (0%)	52	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	128	SER
2	N	29	VAL
1	G	1	GLU
2	V	198	HIS
2	X	211	ARG
2	V	112	ALA
1	J	133	GLY
1	W	1	GLU
1	O	131	THR
1	U	1	GLU

### 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	178/189 (94%)	170 (96%)	8 (4%)	34	59
1	C	179/189 (95%)	170 (95%)	9 (5%)	30	53
1	E	173/189 (92%)	168 (97%)	5 (3%)	50	77
1	G	178/189 (94%)	169 (95%)	9 (5%)	29	52
1	H	179/189 (95%)	173 (97%)	6 (3%)	44	72
1	J	182/189 (96%)	175 (96%)	7 (4%)	40	67
1	M	181/189 (96%)	175 (97%)	6 (3%)	45	73
1	O	183/189 (97%)	175 (96%)	8 (4%)	35	60
1	Q	177/189 (94%)	172 (97%)	5 (3%)	51	78
1	S	177/189 (94%)	168 (95%)	9 (5%)	29	52
1	U	177/189 (94%)	165 (93%)	12 (7%)	20	36
1	W	178/189 (94%)	172 (97%)	6 (3%)	44	72
2	B	185/190 (97%)	171 (92%)	14 (8%)	16	30
2	D	185/190 (97%)	176 (95%)	9 (5%)	31	55
2	F	182/190 (96%)	171 (94%)	11 (6%)	24	43
2	I	185/190 (97%)	175 (95%)	10 (5%)	27	49
2	K	185/190 (97%)	174 (94%)	11 (6%)	24	44
2	L	184/190 (97%)	174 (95%)	10 (5%)	27	49
2	N	185/190 (97%)	174 (94%)	11 (6%)	24	44
2	P	185/190 (97%)	173 (94%)	12 (6%)	21	39
2	R	186/190 (98%)	175 (94%)	11 (6%)	24	44
2	T	185/190 (97%)	174 (94%)	11 (6%)	24	44
2	V	185/190 (97%)	168 (91%)	17 (9%)	11	21
2	X	185/190 (97%)	174 (94%)	11 (6%)	24	44
3	a	12/18 (67%)	11 (92%)	1 (8%)	14	26
3	c	15/18 (83%)	15 (100%)	0	100	100
3	e	13/18 (72%)	13 (100%)	0	100	100
3	g	13/18 (72%)	12 (92%)	1 (8%)	16	30
3	h	12/18 (67%)	12 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	j	18/18 (100%)	15 (83%)	3 (17%)	3	5
3	m	13/18 (72%)	11 (85%)	2 (15%)	3	6
3	o	12/18 (67%)	8 (67%)	4 (33%)	0	0
3	q	18/18 (100%)	15 (83%)	3 (17%)	3	5
3	s	12/18 (67%)	10 (83%)	2 (17%)	3	5
3	u	13/18 (72%)	10 (77%)	3 (23%)	1	1
3	w	12/18 (67%)	11 (92%)	1 (8%)	14	26
All	All	4522/4764 (95%)	4274 (94%)	248 (6%)	27	48

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	28	ASN
1	A	43	LYS
1	A	45	LEU
1	A	73	THR
1	A	82(C)	LEU
1	A	128	SER
1	A	138	LEU
2	B	7	SER
2	B	18	ARG
2	B	24	ARG
2	B	27	GLN
2	B	30	SER
2	B	47	LEU
2	B	72	THR
2	B	76	SER
2	B	125	LEU
2	B	147	GLN
2	B	201	LEU
2	B	210	ASN
2	B	211	ARG
2	B	214	CYS
1	C	28	ASN
1	C	43	LYS
1	C	45	LEU
1	C	73	THR
1	C	82(C)	LEU
1	C	138	LEU

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Mol	Chain	Res	Type
1	C	161	SER
1	C	214	LYS
1	C	215	SER
2	D	24	ARG
2	D	27	GLN
2	D	30	SER
2	D	47	LEU
2	D	72	THR
2	D	125	LEU
2	D	147	GLN
2	D	201	LEU
2	D	210	ASN
1	E	28	ASN
1	E	43	LYS
1	E	45	LEU
1	E	82(C)	LEU
1	E	138	LEU
2	F	7	SER
2	F	27	GLN
2	F	30	SER
2	F	47	LEU
2	F	72	THR
2	F	78	LEU
2	F	125	LEU
2	F	145	LYS
2	F	147	GLN
2	F	201	LEU
2	F	210	ASN
1	G	1	GLU
1	G	28	ASN
1	G	29	VAL
1	G	43	LYS
1	G	45	LEU
1	G	68	THR
1	G	73	THR
1	G	82(C)	LEU
1	G	201	LYS
1	H	28	ASN
1	H	43	LYS
1	H	45	LEU
1	H	82(C)	LEU
1	H	129	LYS

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Mol	Chain	Res	Type
1	H	138	LEU
2	I	7	SER
2	I	24	ARG
2	I	27	GLN
2	I	30	SER
2	I	47	LEU
2	I	72	THR
2	I	125	LEU
2	I	147	GLN
2	I	181	LEU
2	I	210	ASN
1	J	28	ASN
1	J	43	LYS
1	J	45	LEU
1	J	73	THR
1	J	82(C)	LEU
1	J	138	LEU
1	J	192	GLN
2	K	7	SER
2	K	24	ARG
2	K	27	GLN
2	K	30	SER
2	K	47	LEU
2	K	72	THR
2	K	125	LEU
2	K	147	GLN
2	K	201	LEU
2	K	210	ASN
2	K	214	CYS
2	L	7	SER
2	L	24	ARG
2	L	27	GLN
2	L	30	SER
2	L	47	LEU
2	L	72	THR
2	L	125	LEU
2	L	147	GLN
2	L	201	LEU
2	L	210	ASN
1	M	28	ASN
1	M	43	LYS
1	M	45	LEU

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Mol	Chain	Res	Type
1	M	82(C)	LEU
1	M	130	SER
1	M	138	LEU
2	N	7	SER
2	N	24	ARG
2	N	27	GLN
2	N	47	LEU
2	N	72	THR
2	N	125	LEU
2	N	147	GLN
2	N	152	ASN
2	N	201	LEU
2	N	210	ASN
2	N	214	CYS
1	O	11	LEU
1	O	28	ASN
1	O	43	LYS
1	O	45	LEU
1	O	73	THR
1	O	82(C)	LEU
1	O	138	LEU
1	O	214	LYS
2	P	7	SER
2	P	24	ARG
2	P	27	GLN
2	P	30	SER
2	P	47	LEU
2	P	72	THR
2	P	125	LEU
2	P	147	GLN
2	P	152	ASN
2	P	201	LEU
2	P	210	ASN
2	P	213	GLU
1	Q	28	ASN
1	Q	43	LYS
1	Q	45	LEU
1	Q	82(C)	LEU
1	Q	138	LEU
2	R	7	SER
2	R	24	ARG
2	R	27	GLN

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Mol	Chain	Res	Type
2	R	30	SER
2	R	45	LYS
2	R	47	LEU
2	R	125	LEU
2	R	147	GLN
2	R	201	LEU
2	R	210	ASN
2	R	214	CYS
1	S	-1	ILE
1	S	28	ASN
1	S	43	LYS
1	S	45	LEU
1	S	73	THR
1	S	82(C)	LEU
1	S	138	LEU
1	S	195	ILE
1	S	214	LYS
2	T	7	SER
2	T	24	ARG
2	T	27	GLN
2	T	30	SER
2	T	47	LEU
2	T	72	THR
2	T	78	LEU
2	T	125	LEU
2	T	147	GLN
2	T	201	LEU
2	T	210	ASN
1	U	28	ASN
1	U	43	LYS
1	U	45	LEU
1	U	73	THR
1	U	82(C)	LEU
1	U	138	LEU
1	U	184	VAL
1	U	186	SER
1	U	187	SER
1	U	191	THR
1	U	192	GLN
1	U	196	CYS
2	V	7	SER
2	V	24	ARG

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Mol	Chain	Res	Type
2	V	27	GLN
2	V	30	SER
2	V	47	LEU
2	V	72	THR
2	V	109	THR
2	V	125	LEU
2	V	147	GLN
2	V	181	LEU
2	V	195	GLU
2	V	197	THR
2	V	199	GLN
2	V	201	LEU
2	V	202	SER
2	V	203	SER
2	V	210	ASN
1	W	28	ASN
1	W	43	LYS
1	W	45	LEU
1	W	73	THR
1	W	82(C)	LEU
1	W	138	LEU
2	X	7	SER
2	X	27	GLN
2	X	30	SER
2	X	47	LEU
2	X	72	THR
2	X	125	LEU
2	X	147	GLN
2	X	201	LEU
2	X	210	ASN
2	X	213	GLU
2	X	214	CYS
3	a	5	LEU
3	g	5	LEU
3	j	5	LEU
3	j	15	VAL
3	j	17	HIS
3	m	9	LEU
3	m	10	LEU
3	o	5	LEU
3	o	8	LEU
3	o	9	LEU

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Mol	Chain	Res	Type
3	o	10	LEU
3	q	5	LEU
3	q	15	VAL
3	q	17	HIS
3	s	9	LEU
3	s	10	LEU
3	u	5	LEU
3	u	9	LEU
3	u	12	LEU
3	w	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	171	GLN
1	A	197	ASN
1	A	200	HIS
2	B	27	GLN
2	B	155	GLN
2	B	210	ASN
1	C	28	ASN
1	C	171	GLN
1	C	197	ASN
1	C	200	HIS
2	D	6	GLN
2	D	27	GLN
2	D	147	GLN
2	D	155	GLN
2	D	210	ASN
1	E	28	ASN
1	E	171	GLN
1	E	197	ASN
1	E	200	HIS
2	F	27	GLN
2	F	155	GLN
2	F	210	ASN
1	G	28	ASN
1	G	171	GLN
1	G	197	ASN
1	G	199	ASN
1	G	200	HIS

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Mol	Chain	Res	Type
1	H	28	ASN
1	H	171	GLN
1	H	197	ASN
1	H	200	HIS
2	I	27	GLN
2	I	147	GLN
2	I	155	GLN
2	I	160	GLN
2	I	210	ASN
1	J	28	ASN
1	J	171	GLN
1	J	197	ASN
1	J	200	HIS
2	K	27	GLN
2	K	137	ASN
2	K	147	GLN
2	K	155	GLN
2	K	210	ASN
2	L	27	GLN
2	L	155	GLN
2	L	160	GLN
2	L	210	ASN
1	M	28	ASN
1	M	171	GLN
1	M	197	ASN
1	M	200	HIS
2	N	27	GLN
2	N	155	GLN
2	N	210	ASN
1	O	28	ASN
1	O	171	GLN
1	O	197	ASN
1	O	200	HIS
2	P	27	GLN
2	P	147	GLN
2	P	155	GLN
1	Q	28	ASN
1	Q	171	GLN
1	Q	197	ASN
1	Q	200	HIS
2	R	27	GLN
2	R	155	GLN

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Mol	Chain	Res	Type
2	R	198	HIS
2	R	210	ASN
1	S	28	ASN
1	S	171	GLN
1	S	197	ASN
1	S	200	HIS
2	T	27	GLN
2	T	155	GLN
2	T	210	ASN
1	U	28	ASN
1	U	171	GLN
1	U	197	ASN
1	U	200	HIS
2	V	27	GLN
2	V	155	GLN
2	V	199	GLN
2	V	210	ASN
1	W	28	ASN
1	W	171	GLN
1	W	197	ASN
1	W	199	ASN
1	W	200	HIS
2	X	27	GLN
2	X	155	GLN
2	X	210	ASN
3	j	16	GLN
3	q	16	GLN
3	q	17	HIS
3	u	13	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

15 ligands are modelled in this entry.

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	NO3	B	301	-	1,3,3	0.30	0	0,3,3	0.00	-
4	NO3	D	301	-	1,3,3	0.26	0	0,3,3	0.00	-
4	NO3	F	301	-	1,3,3	0.39	0	0,3,3	0.00	-
4	NO3	I	301	-	1,3,3	0.35	0	0,3,3	0.00	-
4	NO3	K	301	-	1,3,3	0.55	0	0,3,3	0.00	-
4	NO3	L	301	-	1,3,3	0.19	0	0,3,3	0.00	-
5	EDO	N	301	-	3,3,3	0.52	0	2,2,2	0.12	0
4	NO3	N	302	-	1,3,3	0.52	0	0,3,3	0.00	-
4	NO3	P	301	-	1,3,3	0.25	0	0,3,3	0.00	-
5	EDO	Q	301	-	3,3,3	0.44	0	2,2,2	0.21	0
4	NO3	R	301	-	1,3,3	0.39	0	0,3,3	0.00	-
4	NO3	T	301	-	1,3,3	0.53	0	0,3,3	0.00	-
4	NO3	V	301	-	1,3,3	0.31	0	0,3,3	0.00	-
5	EDO	W	301	-	3,3,3	0.31	0	2,2,2	0.55	0
4	NO3	X	301	-	1,3,3	0.36	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NO3	B	301	-	-	0/0/0/0	0/0/0/0
4	NO3	D	301	-	-	0/0/0/0	0/0/0/0
4	NO3	F	301	-	-	0/0/0/0	0/0/0/0
4	NO3	I	301	-	-	0/0/0/0	0/0/0/0
4	NO3	K	301	-	-	0/0/0/0	0/0/0/0
4	NO3	L	301	-	-	0/0/0/0	0/0/0/0
5	EDO	N	301	-	-	0/1/1/1	0/0/0/0
4	NO3	N	302	-	-	0/0/0/0	0/0/0/0
4	NO3	P	301	-	-	0/0/0/0	0/0/0/0
5	EDO	Q	301	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NO3	R	301	-	-	0/0/0/0	0/0/0/0
4	NO3	T	301	-	-	0/0/0/0	0/0/0/0
4	NO3	V	301	-	-	0/0/0/0	0/0/0/0
5	EDO	W	301	-	-	0/1/1/1	0/0/0/0
4	NO3	X	301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	301	NO3	1	0
4	X	301	NO3	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	A	217/229 (94%)	0.08	0 100 100	30, 45, 74, 109	0
1	C	219/229 (95%)	0.10	2 (0%) 85 88	24, 36, 67, 108	0
1	E	212/229 (92%)	0.76	29 (13%) 4 4	38, 61, 111, 133	0
1	G	218/229 (95%)	0.11	5 (2%) 64 67	29, 39, 59, 122	0
1	H	219/229 (95%)	0.08	1 (0%) 91 92	25, 36, 62, 81	0
1	J	224/229 (97%)	0.31	8 (3%) 46 51	27, 46, 90, 110	0
1	M	220/229 (96%)	0.08	4 (1%) 71 75	24, 36, 59, 109	0
1	O	223/229 (97%)	0.22	4 (1%) 71 75	36, 47, 76, 108	0
1	Q	217/229 (94%)	0.12	4 (1%) 71 75	24, 40, 75, 101	0
1	S	215/229 (93%)	0.26	9 (4%) 40 45	30, 49, 91, 113	0
1	U	217/229 (94%)	0.87	41 (18%) 2 1	34, 52, 125, 144	0
1	W	218/229 (95%)	0.15	3 (1%) 78 80	31, 44, 63, 118	0
2	B	210/215 (97%)	0.25	4 (1%) 70 73	42, 56, 73, 101	0
2	D	210/215 (97%)	0.15	4 (1%) 70 73	30, 42, 61, 101	0
2	F	207/215 (96%)	0.78	23 (11%) 7 7	45, 71, 97, 107	0
2	I	211/215 (98%)	0.15	5 (2%) 62 66	31, 42, 63, 104	0
2	K	210/215 (97%)	0.27	1 (0%) 91 92	29, 48, 72, 97	0
2	L	209/215 (97%)	0.16	3 (1%) 78 80	31, 43, 61, 93	0
2	N	210/215 (97%)	0.18	2 (0%) 84 86	30, 41, 60, 90	0
2	P	210/215 (97%)	0.29	5 (2%) 62 66	32, 50, 74, 90	0
2	R	211/215 (98%)	0.11	4 (1%) 70 73	25, 39, 61, 107	0
2	T	210/215 (97%)	0.52	16 (7%) 17 18	38, 59, 82, 111	0
2	V	210/215 (97%)	0.91	26 (12%) 5 5	50, 69, 99, 114	0
2	X	210/215 (97%)	0.17	4 (1%) 70 73	33, 45, 68, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	a	12/19 (63%)	1.53	5 (41%) 0 0	64, 75, 88, 94	0
3	c	16/19 (84%)	1.35	4 (25%) 1 1	57, 75, 101, 107	0
3	e	13/19 (68%)	0.77	0 100 100	57, 68, 85, 90	0
3	g	13/19 (68%)	1.05	1 (7%) 16 18	60, 71, 88, 93	0
3	h	12/19 (63%)	2.02	6 (50%) 0 0	77, 87, 97, 99	0
3	j	19/19 (100%)	0.98	3 (15%) 3 2	43, 55, 83, 89	0
3	m	13/19 (68%)	0.39	0 100 100	51, 59, 72, 80	0
3	o	12/19 (63%)	1.62	5 (41%) 0 0	88, 96, 107, 113	0
3	q	19/19 (100%)	0.86	2 (10%) 8 8	42, 53, 79, 80	0
3	s	12/19 (63%)	0.63	1 (8%) 14 15	51, 65, 86, 86	0
3	u	13/19 (68%)	1.37	3 (23%) 1 1	76, 84, 99, 124	0
3	w	12/19 (63%)	0.88	0 100 100	72, 83, 95, 105	0
All	All	5303/5556 (95%)	0.32	237 (4%) 37 42	24, 46, 88, 144	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	136	ALA	11.0
1	J	-1	ILE	7.9
1	S	215	SER	7.8
1	U	161	SER	7.5
2	V	214	CYS	6.6
2	V	5	THR	6.5
1	J	191	THR	6.4
2	I	212	GLY	6.2
1	U	194	TYR	6.2
1	G	133	GLY	5.9
1	U	137	ALA	5.7
2	F	192	TYR	5.6
1	U	154	TRP	5.6
1	O	0	SER	5.5
1	U	135	THR	5.5
2	X	5	THR	5.5
1	U	138	LEU	5.5
1	U	133	GLY	5.4
1	U	162	GLY	5.2
2	P	214	CYS	5.2
1	G	216	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	J	132	SER	5.0
2	N	5	THR	4.8
1	E	121	VAL	4.8
1	M	0	SER	4.7
2	B	5	THR	4.7
1	E	136	ALA	4.7
1	E	135	THR	4.7
3	u	13	ASN	4.6
1	W	216	CYS	4.6
1	U	191	THR	4.6
1	W	0	SER	4.5
1	U	125	ALA	4.4
1	E	124	LEU	4.4
1	U	215	SER	4.4
2	V	142	ARG	4.4
2	R	30	SER	4.3
2	B	29	VAL	4.3
2	K	5	THR	4.2
2	T	193	ALA	4.2
2	R	4	MET	4.1
2	L	29	VAL	4.0
1	E	125	ALA	4.0
1	Q	217	ASP	4.0
2	V	29	VAL	4.0
1	O	132	SER	4.0
1	W	215	SER	3.9
3	o	10	LEU	3.9
3	q	14	ALA	3.9
1	E	185	PRO	3.9
2	N	29	VAL	3.8
1	E	194	TYR	3.8
1	E	190	GLY	3.8
1	E	189	LEU	3.7
2	F	190	LYS	3.7
2	P	29	VAL	3.7
1	Q	0	SER	3.6
1	U	184	VAL	3.6
2	L	5	THR	3.6
1	U	152	VAL	3.6
1	U	206	LYS	3.6
1	O	216	CYS	3.6
1	E	138	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	204	ASN	3.5
1	U	158	ALA	3.5
1	G	0	SER	3.5
1	E	122	PHE	3.5
2	T	214	CYS	3.5
2	F	5	THR	3.5
3	a	7	ARG	3.5
2	V	106	ILE	3.5
2	D	5	THR	3.5
2	I	4	MET	3.5
1	U	216	CYS	3.4
2	F	127	SER	3.4
1	U	183	THR	3.4
2	I	5	THR	3.4
2	V	141	PRO	3.4
2	T	190	LYS	3.3
2	V	111	ALA	3.3
1	E	206	LYS	3.3
1	E	191	THR	3.2
1	J	131	THR	3.2
2	F	191	VAL	3.2
2	T	30	SER	3.2
1	U	182	VAL	3.2
2	F	116	PHE	3.1
1	U	0	SER	3.1
2	V	140	TYR	3.1
2	V	116	PHE	3.1
3	h	1	ASN	3.1
3	j	17	HIS	3.1
2	F	153	ALA	3.1
1	U	193	THR	3.0
2	D	30	SER	3.0
3	o	12	LEU	3.0
1	U	198	VAL	3.0
2	X	214	CYS	3.0
2	F	205	VAL	3.0
1	U	160	THR	3.0
2	V	137	ASN	3.0
2	R	29	VAL	2.9
1	U	134	GLY	2.9
1	S	211	VAL	2.9
3	h	7	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	V	110	VAL	2.9
1	E	134	GLY	2.9
2	F	150	VAL	2.9
1	E	195	ILE	2.9
1	G	214	LYS	2.9
2	V	14	SER	2.8
1	U	195	ILE	2.8
2	T	202	SER	2.8
2	L	30	SER	2.8
3	c	15	VAL	2.8
1	U	212	GLU	2.8
1	J	190	GLY	2.8
1	E	0	SER	2.8
1	C	217	ASP	2.8
3	h	4	GLU	2.8
2	F	122	ASP	2.8
1	E	207	VAL	2.7
2	P	5	THR	2.7
2	F	115	VAL	2.7
2	V	202	SER	2.7
2	F	149	LYS	2.7
1	U	214	LYS	2.7
2	V	172	THR	2.6
1	U	155	ASN	2.6
1	M	128	SER	2.6
2	T	153	ALA	2.6
1	G	215	SER	2.6
2	F	197	THR	2.5
2	F	206	THR	2.5
2	R	5	THR	2.5
3	s	12	LEU	2.5
3	a	1	ASN	2.5
2	X	213	GLU	2.5
2	V	78	LEU	2.5
3	c	13	ASN	2.5
3	g	11	GLU	2.5
1	E	157	GLY	2.5
1	Q	134	GLY	2.5
1	O	206	LYS	2.5
1	H	0	SER	2.4
1	Q	215	SER	2.4
2	V	13	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	V	54	LEU	2.4
1	U	208	ASP	2.4
3	h	6	ASP	2.4
2	T	205	VAL	2.4
1	E	188	SER	2.4
2	P	30	SER	2.4
3	j	12	LEU	2.4
1	U	211	VAL	2.4
1	S	-1	ILE	2.4
3	a	12	LEU	2.4
3	u	12	LEU	2.4
1	J	29	VAL	2.4
1	U	210	LYS	2.4
2	F	179	LEU	2.4
1	E	177	SER	2.4
1	E	158	ALA	2.3
1	U	159	LEU	2.3
2	T	201	LEU	2.3
3	j	18	ASN	2.3
3	q	12	LEU	2.3
1	U	213	PRO	2.3
1	S	137	ALA	2.3
1	J	209	LYS	2.3
1	S	210	LYS	2.3
2	B	212	GLY	2.3
2	V	175	LEU	2.3
2	F	209	PHE	2.3
1	J	0	SER	2.3
1	S	122	PHE	2.3
3	h	5	LEU	2.3
2	I	29	VAL	2.3
2	V	139	PHE	2.3
3	a	8	LEU	2.3
3	h	12	LEU	2.3
2	T	152	ASN	2.2
1	M	217	ASP	2.2
2	V	104	VAL	2.2
1	S	191	THR	2.2
2	F	126	LYS	2.2
2	T	212	GLY	2.2
2	B	76	SER	2.2
2	D	29	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	196	CYS	2.2
2	T	5	THR	2.2
1	S	141	LEU	2.2
3	c	12	LEU	2.2
3	o	1	ASN	2.2
1	C	161	SER	2.2
2	T	126	LYS	2.2
2	P	68	GLY	2.2
3	a	10	LEU	2.2
2	F	203	SER	2.2
1	E	198	VAL	2.2
2	I	106	ILE	2.2
2	F	200	GLY	2.2
2	D	214	CYS	2.2
1	U	164	HIS	2.1
2	F	189	HIS	2.1
2	V	114	SER	2.1
3	c	14	ALA	2.1
2	V	83	PHE	2.1
1	M	1	GLU	2.1
1	U	157	GLY	2.1
2	T	112	ALA	2.1
1	E	175	LEU	2.1
1	E	187	SER	2.1
3	o	7	ARG	2.1
1	U	207	VAL	2.1
2	T	184	ALA	2.1
2	V	144	ALA	2.1
1	U	189	LEU	2.1
2	F	154	LEU	2.1
1	U	127	SER	2.1
1	U	199	ASN	2.1
2	V	138	ASN	2.1
2	X	29	VAL	2.1
3	o	4	GLU	2.1
1	U	192	GLN	2.1
1	E	123	PRO	2.1
1	E	142	VAL	2.1
1	E	184	VAL	2.1
2	V	6	GLN	2.1
1	U	185	PRO	2.0
2	V	146	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	155	GLN	2.0
2	T	31	SER	2.0
1	S	189	LEU	2.0
3	u	8	LEU	2.0
2	F	188	LYS	2.0
2	T	198	HIS	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NO3	V	301	4/4	0.80	0.61	13.87	37,39,39,39	4
4	NO3	K	301	4/4	0.95	0.30	7.08	41,42,42,47	0
4	NO3	P	301	4/4	0.92	0.30	6.77	30,31,31,32	4
4	NO3	D	301	4/4	0.98	0.27	6.36	41,45,45,47	0
4	NO3	B	301	4/4	0.84	0.30	6.03	59,59,63,66	0
5	EDO	Q	301	4/4	0.95	0.26	5.91	32,33,33,33	0
4	NO3	T	301	4/4	0.97	0.30	5.63	22,23,23,23	4
4	NO3	F	301	4/4	0.93	0.32	5.41	26,26,27,28	4
4	NO3	L	301	4/4	0.87	0.30	5.30	26,26,27,27	4
4	NO3	R	301	4/4	0.98	0.19	1.92	38,38,38,39	0
4	NO3	I	301	4/4	0.93	0.20	1.67	49,49,52,55	0
4	NO3	X	301	4/4	0.96	0.17	1.44	47,49,49,50	0
5	EDO	N	301	4/4	0.91	0.16	-0.28	38,39,39,40	0
4	NO3	N	302	4/4	0.98	0.14	-0.45	41,42,43,45	0
5	EDO	W	301	4/4	0.74	0.24	-	47,47,48,48	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.