Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 07:42 PM EDT

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*
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:

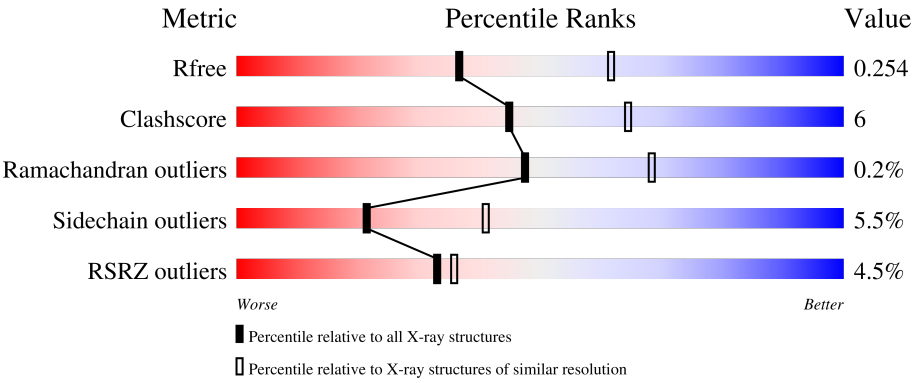
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	86% 9% 5%
1	C	229	% 84% 10%
1	E	229	13% 83% 9% 7%
1	G	229	2% 86% 8% 5%
1	H	229	85% 9%

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Mol	Chain	Length	Quality of chain
1	J	229	3% 86% 11%
1	M	229	2% 82% 14%
1	O	229	2% 86% 10%
1	Q	229	2% 86% 7% 5%
1	S	229	4% 83% 9% 6%
1	U	229	19% 78% 15% 5%
1	W	229	86% 9% 5%
2	B	215	2% 85% 10%
2	D	215	2% 86% 9%
2	F	215	11% 82% 11%
2	I	215	2% 86% 10%
2	K	215	85% 11%
2	L	215	85% 10%
2	N	215	81% 13%
2	P	215	3% 83% 12%
2	R	215	2% 80% 16%
2	T	215	7% 81% 15%
2	V	215	12% 77% 15% 6%
2	X	215	2% 82% 12%
3	a	19	26% 53% 11% 37%
3	c	19	16% 84% 16%
3	e	19	68% 32%
3	g	19	5% 63% 5% 32%
3	h	19	32% 63% 37%
3	j	19	16% 84% 16%

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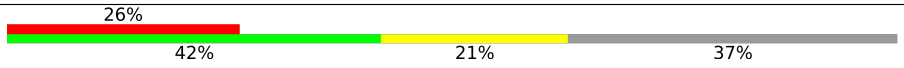
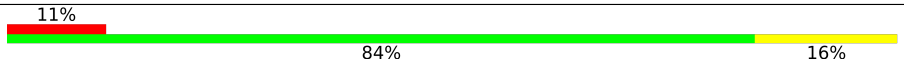
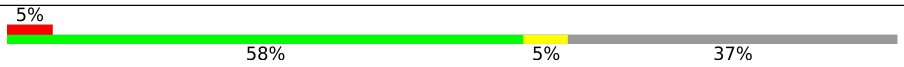
Mol	Chain	Length	Quality of chain
3	m	19	
3	o	19	
3	q	19	
3	s	19	
3	u	19	
3	w	19	

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	V	301	-	-	-	X

2 Entry composition (i)

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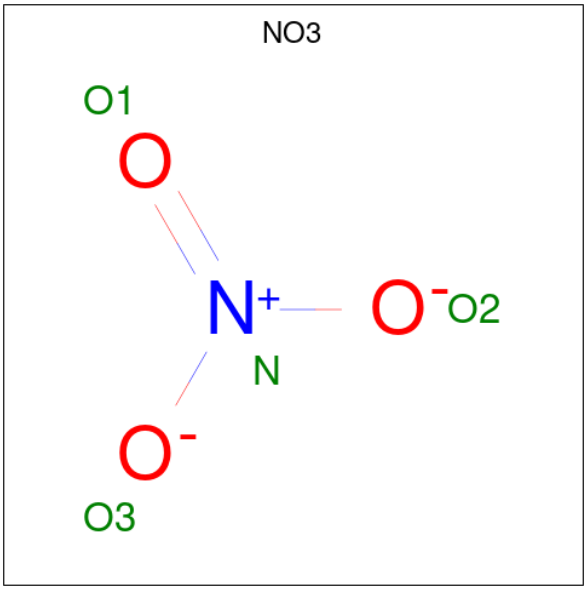
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	s	12	Total C N O 99 63 16 20	0	0	0
3	u	13	Total C N O 107 67 18 22	0	0	0
3	w	12	Total C N O 99 63 16 20	0	0	0

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



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

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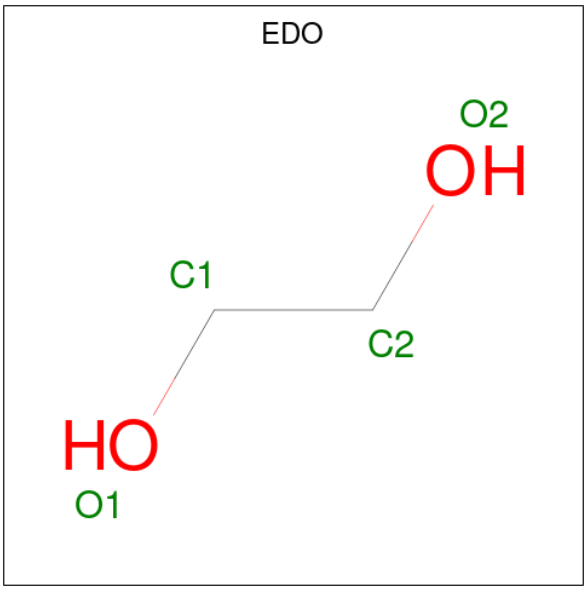
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	R	1	Total N O 4 1 3	0	0
4	T	1	Total N O 4 1 3	0	0
4	V	1	Total N O 4 1 3	0	0
4	X	1	Total N O 4 1 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

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

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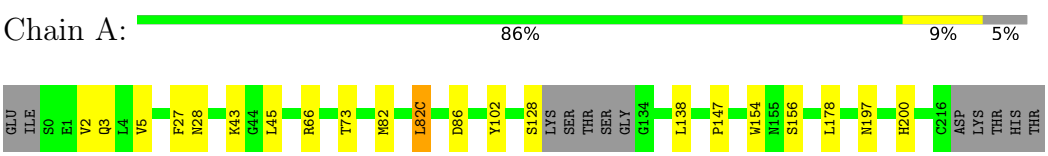
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	X	12	Total O 12 12	0	0
6	a	1	Total O 1 1	0	0
6	c	1	Total O 1 1	0	0
6	e	1	Total O 1 1	0	0
6	g	2	Total O 2 2	0	0
6	j	4	Total O 4 4	0	0
6	m	1	Total O 1 1	0	0
6	o	1	Total O 1 1	0	0
6	q	3	Total O 3 3	0	0
6	s	1	Total O 1 1	0	0
6	u	1	Total O 1 1	0	0
6	w	1	Total O 1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

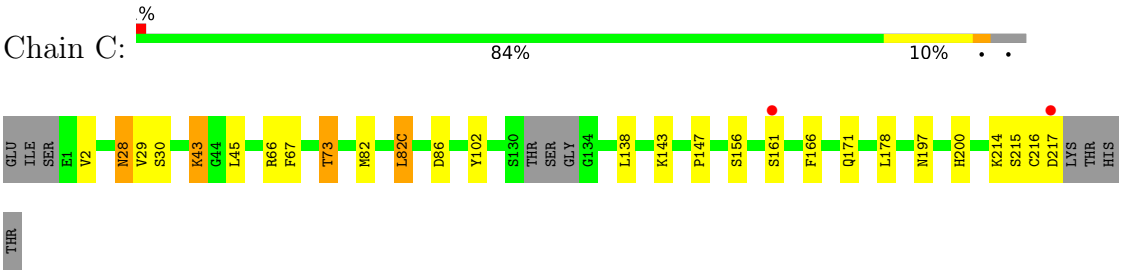
- Molecule 1: FAB HEAVY CHAIN

Chain A:



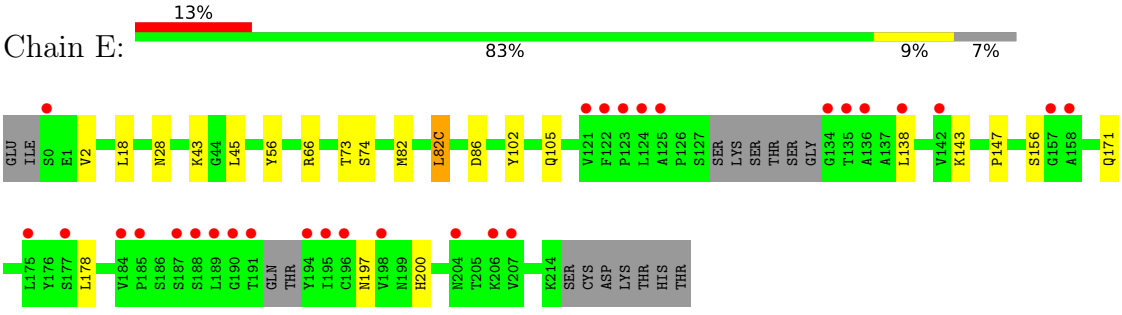
- Molecule 1: FAB HEAVY CHAIN

Chain C:



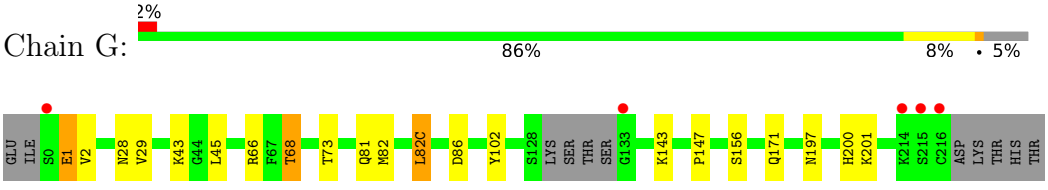
- Molecule 1: FAB HEAVY CHAIN

Chain E:



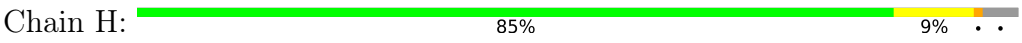
- Molecule 1: FAB HEAVY CHAIN

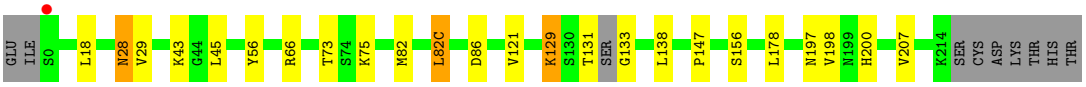
Chain G:



- Molecule 1: FAB HEAVY CHAIN

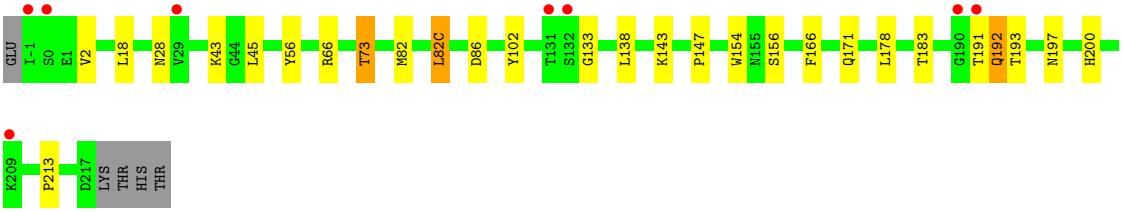
Chain H:





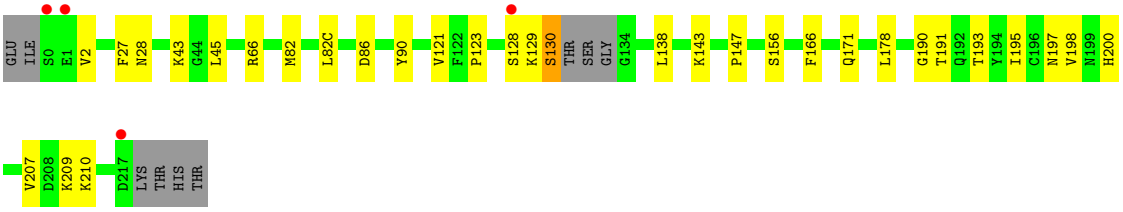
• Molecule 1: FAB HEAVY CHAIN

Chain J:



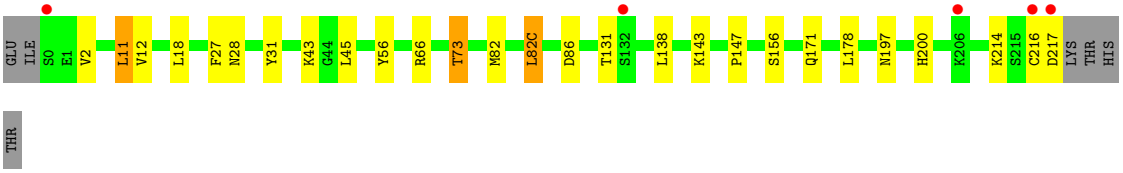
• Molecule 1: FAB HEAVY CHAIN

Chain M:



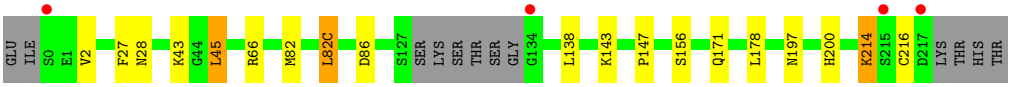
• Molecule 1: FAB HEAVY CHAIN

Chain O:



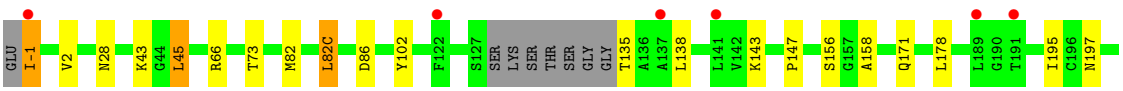
• Molecule 1: FAB HEAVY CHAIN

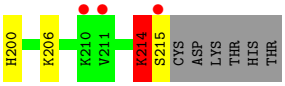
Chain Q:



• Molecule 1: FAB HEAVY CHAIN

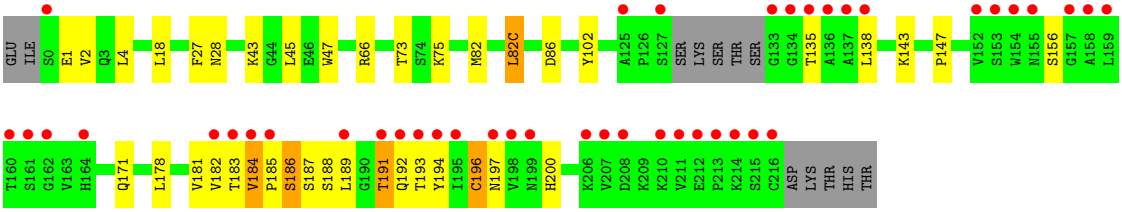
Chain S:





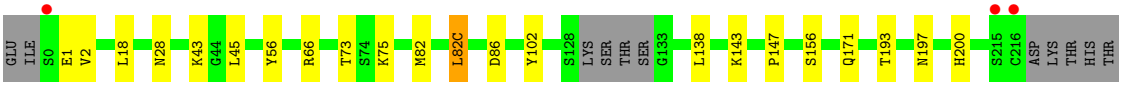
• Molecule 1: FAB HEAVY CHAIN

Chain U:



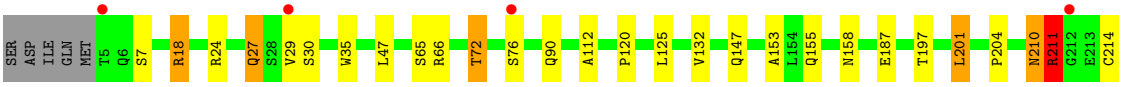
• Molecule 1: FAB HEAVY CHAIN

Chain W:



• Molecule 2: FAB LIGHT CHAIN

Chain B:

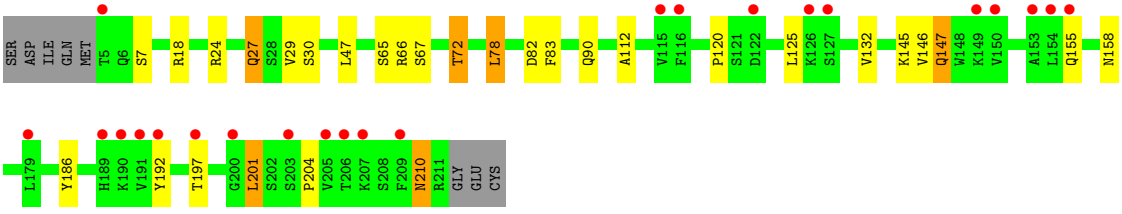


• Molecule 2: FAB LIGHT CHAIN

Chain D:

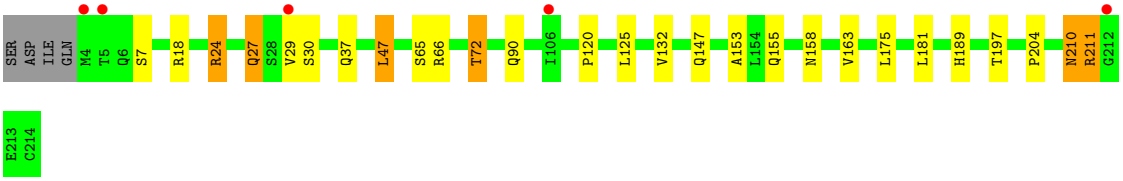
• Molecule 2: FAB LIGHT CHAIN

Chain F:



• Molecule 2: FAB LIGHT CHAIN

Chain I:

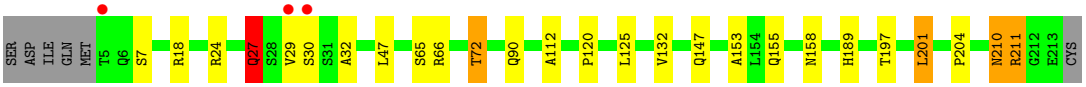


• Molecule 2: FAB LIGHT CHAIN

Chain K:

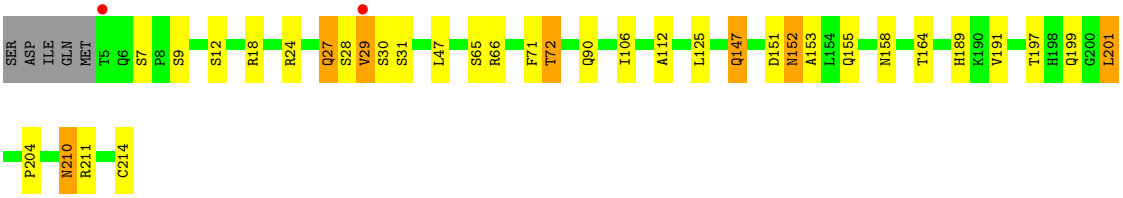
• Molecule 2: FAB LIGHT CHAIN

Chain L:



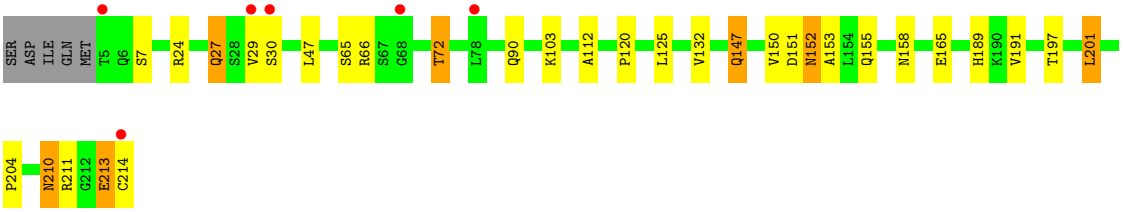
• Molecule 2: FAB LIGHT CHAIN

Chain N:



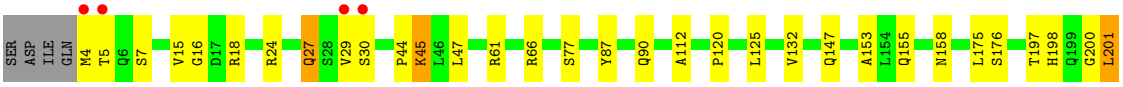
• Molecule 2: FAB LIGHT CHAIN

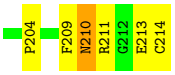
Chain P:



• Molecule 2: FAB LIGHT CHAIN

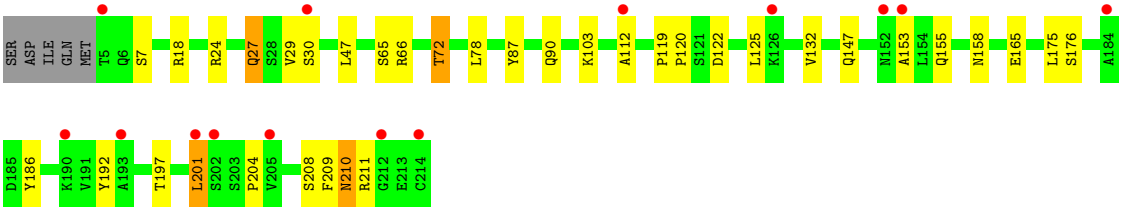
Chain R:





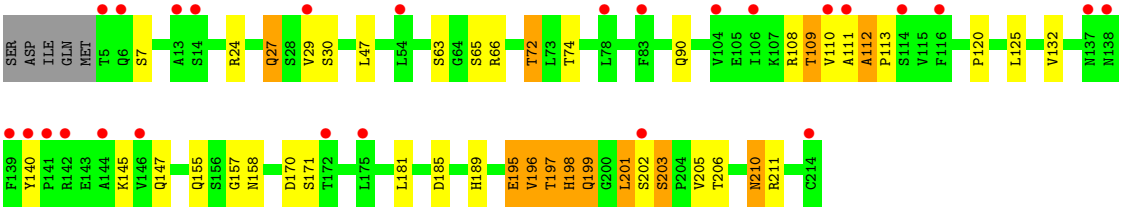
• Molecule 2: FAB LIGHT CHAIN

Chain T:



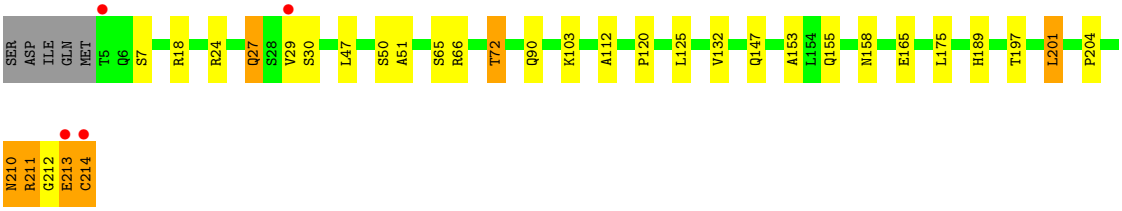
• Molecule 2: FAB LIGHT CHAIN

Chain V:



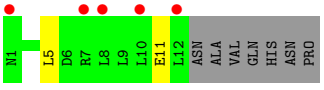
• Molecule 2: FAB LIGHT CHAIN

Chain X:



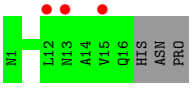
• Molecule 3: PAXILLIN LD2

Chain a:



• Molecule 3: PAXILLIN LD2

Chain c:

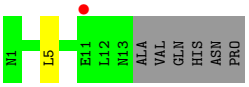


• Molecule 3: PAXILLIN LD2

Chain e:

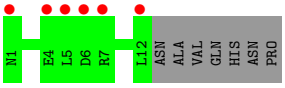
• Molecule 3: PAXILLIN LD2

Chain g:



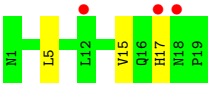
• Molecule 3: PAXILLIN LD2

Chain h:



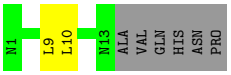
• Molecule 3: PAXILLIN LD2

Chain j:



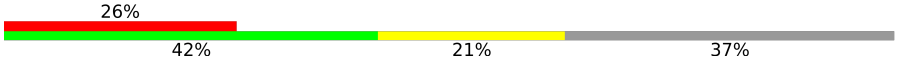
• Molecule 3: PAXILLIN LD2

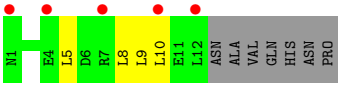
Chain m:



• Molecule 3: PAXILLIN LD2

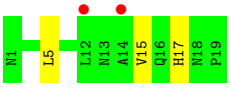
Chain o:





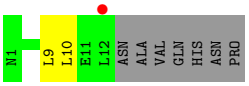
• Molecule 3: PAXILLIN LD2

Chain q:



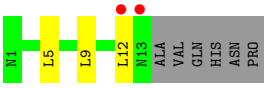
• Molecule 3: PAXILLIN LD2

Chain s:



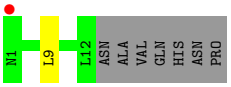
• Molecule 3: PAXILLIN LD2

Chain u:



• Molecule 3: PAXILLIN LD2

Chain w:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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) 94.3 (100.11-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	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	9883 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	40426	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:HD13	2:V:201:LEU:O	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:O	2:V:195:GLU:HG3	1.68	0.93
2:V:201:LEU:HD13	2:V:201:LEU:C	1.89	0.92
1:U:185:PRO:CG	1:U:188:SER:HB2	2.01	0.90
1:S:-1:ILE:O	1:S:-1:ILE:HG23	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:O	2:V:201:LEU:CD1	2.30	0.79
1:S:-1:ILE:O	1:S:-1:ILE:CG2	2.30	0.78
2:V:201:LEU:CD2	2:V:203:SER:O	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
2:L:155:GLN:HE21	2:L:158:ASN:HD21	1.31	0.77
1:M:193:THR:HG21	2:R:16:GLY:HA2	1.66	0.77
2:N:155:GLN:HE21	2:N:158:ASN:HD21	1.30	0.77
2:N:210:ASN:OD1	2:P:151:ASP:HB3	1.85	0.77
2:V:111:ALA:O	2:V:112:ALA:CB	2.30	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:A:82:MET:HE2	1:A:82(C):LEU:HD11	1.66	0.76
1:M:195:ILE:CD1	2:R:15:VAL:CG1	2.56	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
2:B:197:THR:HG23	6:B:401:HOH:O	1.90	0.71
1:E:74:SER:HB2	1:S:158:ALA:O	1.89	0.71
1:G:82:MET:HE2	1:G:82(C):LEU:HD11	1.71	0.71
2:R:197:THR:HG23	6:R:403:HOH:O	1.90	0.71
1:C:156:SER:H	1:C:197:ASN:HD21	1.37	0.70
2:V:195:GLU:O	2:V:195:GLU:CG	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:D:211:ARG:NH1	2:D:211:ARG:HG2	2.10	0.67
2:V:63:SER:OG	2:V:74:THR:CG2	2.42	0.67
2:I:153:ALA:HB2	2:R:18:ARG:HD3	1.76	0.66
1:H:75:LYS:NZ	1:J:73:THR:HB	2.10	0.66
1:H:121:VAL:HG21	1:H:207:VAL:CG1	2.26	0.66
1:S:214:LYS:NZ	2:T:122:ASP:OD2	2.29	0.66
2:B:155:GLN:HE21	2:B:158:ASN:HD21	1.42	0.65
2:P:213:GLU:HG2	2:P:214:CYS:N	2.09	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
1:M:129:LYS:H	1:M:130:SER:C	2.00	0.65
2:V:108:ARG:HD2	2:V:171:SER:HB2	1.79	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
1:O:31:TYR:CE1	1:S:206:LYS:NZ	2.65	0.64
2:P:155:GLN:HE21	2:P:158:ASN:HD21	1.45	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
2:P:152:ASN:OD1	2:P:152:ASN:C	2.39	0.61
1:U:184:VAL:HB	1:U:185:PRO:HD2	1.82	0.61
1:O:11:LEU:HD22	1:O:12:VAL:N	2.16	0.61
2:X:210:ASN:N	2:X:210:ASN:HD22	1.98	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:C	2:N:152:ASN:OD1	2.40	0.60
2:V:197:THR:O	2:V:198:HIS:HB2	1.99	0.60
2:D:153:ALA:HB2	2:N:18:ARG:HD3	1.83	0.60
1:M:121:VAL:CG2	1:M:207:VAL:HG11	2.32	0.60
1:U:185:PRO:HG2	1:U:188:SER:HB3	1.79	0.60
1:M:121:VAL:HG21	1:M:207:VAL:CG1	2.31	0.60
2:B:210:ASN:N	2:B:210:ASN:HD22	1.98	0.60
2:B:153:ALA:HB2	2:T:18:ARG:HD3	1.83	0.60
2:N:210:ASN:N	2:N:210:ASN:HD22	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:C	1:S:178:LEU:HD12	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
1:H:129:LYS:O	1:H:129:LYS:HG2	2.05	0.57
2:N:151:ASP:HB3	2:P:210:ASN:OD1	2.04	0.57
2:V:145:LYS:HE2	2:V:197:THR:HG21	1.87	0.57
2:F:29:VAL:HG13	2:F:66:ARG:HH21	1.69	0.57
1:S:2:VAL:HG11	1:S:102:TYR:CE2	2.38	0.57
1:O:82:MET:HE2	1:O:82(C):LEU:HD11	1.87	0.57
2:T:112:ALA:HB1	2:T:201:LEU:CD1	2.34	0.57
2:V:113:PRO:HD3	2:V:198:HIS:CE1	2.39	0.57
1:M:82:MET:HE3	1:M:90:TYR:CE2	2.40	0.56
2:R:210:ASN:N	2:R:210:ASN:HD22	2.02	0.56
1:U:184:VAL:CB	1:U:194:TYR:CZ	2.87	0.56
2:I:155:GLN:HE21	2:I:158:ASN:HD21	1.52	0.56
2:L:210:ASN:N	2:L:210:ASN:HD22	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:C:2:VAL:HG11	1:C:102:TYR:CZ	2.40	0.56
2:D:65:SER:HB3	2:D:72:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:184:VAL:HG23	1:U:185:PRO:HD2	1.88	0.56
2:V:113:PRO:HG3	2:V:198:HIS:CE1	2.41	0.56
2:B:65:SER:HB3	2:B:72:THR:HG22	1.88	0.56
1:M:210:LYS:O	1:M:210:LYS:HG3	2.06	0.56
1:S:2:VAL:HG11	1:S:102:TYR:CZ	2.40	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
1:A:178:LEU:HD12	1:A:178:LEU:C	2.27	0.55
2:P:65:SER:HB3	2:P:72:THR:HG22	1.89	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:U:66:ARG:NH2	1:U:86:ASP:OD2	2.40	0.55
1:W:2:VAL:HG11	1:W:102:TYR:CZ	2.42	0.55
2:D:29:VAL:HG13	2:D:66:ARG:HH21	1.71	0.55
2:V:196:VAL:HG12	2:V:197:THR:O	2.06	0.55
2:D:199:GLN:HA	2:N:199:GLN:HG3	1.89	0.55
1:E:2:VAL:HG11	1:E:102:TYR:CZ	2.42	0.55
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.40	0.55
2:L:65:SER:HB3	2:L:72:THR:HG22	1.89	0.55
1:H:178:LEU:HD12	1:H:178:LEU:C	2.27	0.54
1:O:66:ARG:NH2	1:O:86:ASP:OD2	2.40	0.54
1:Q:66:ARG:NH2	1:Q:86:ASP:OD2	2.40	0.54
1:W:66:ARG:NH2	1:W:86:ASP:OD2	2.41	0.54
1:C:2:VAL:CG1	1:C:102:TYR:CZ	2.90	0.54
1:H:18:LEU:HD13	1:J:56:TYR:CE1	2.42	0.54
2:K:65:SER:HB3	2:K:72:THR:HG22	1.88	0.54
2:I:65:SER:HB3	2:I:72:THR:HG22	1.90	0.54
2:V:65:SER:HB3	2:V:72:THR:HG22	1.89	0.54
1:A:2:VAL:HG11	1:A:102:TYR:CE2	2.42	0.54
1:A:66:ARG:NH2	1:A:86:ASP:OD2	2.40	0.54
2:F:65:SER:HB3	2:F:72:THR:HG22	1.89	0.54
1:J:66:ARG:NH2	1:J: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
1:G:66:ARG:NH2	1:G:86:ASP:OD2	2.41	0.54
2:K:18:ARG:HD3	2:P:153:ALA:HB2	1.90	0.54
2:P:210:ASN:N	2:P:210:ASN:HD22	2.05	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
1:A:2:VAL:HG11	1:A:102:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:27:GLN:HE21	2:L:27:GLN:CA	2.21	0.53
1:M:178:LEU:HD12	1:M:178:LEU:C	2.28	0.53
1:Q:178:LEU:C	1:Q:178:LEU:HD12	2.29	0.53
1:U:2:VAL:HG11	1:U:102:TYR:CZ	2.44	0.53
2:F:155:GLN:HE21	2:F:158:ASN:HD21	1.55	0.53
2:L:112:ALA:HB1	2:L:201:LEU:CD1	2.38	0.53
1:S:2:VAL:CG1	1:S:102:TYR:CZ	2.91	0.53
1:U:184:VAL:CG1	1:U:194:TYR:CE1	2.83	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
2:L:27:GLN:HB3	2:L:90:GLN:HG3	1.90	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: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:S:2:VAL:HG13	1:S:102:TYR:CE1	2.44	0.53
1:E:2:VAL:CG1	1:E:102:TYR:CZ	2.92	0.53
2:L:18:ARG:HD3	2:X:153:ALA:HB2	1.89	0.52
2:P:189:HIS:O	2:P:211:ARG:NH1	2.42	0.52
2:X:112:ALA:HB1	2:X:201:LEU:CD1	2.40	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:I:189:HIS:O	2:I:211:ARG:NH1	2.42	0.52
2:X:189:HIS:O	2:X: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:O	1:H:129:LYS:CG	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:G:2:VAL:HG13	1:G:102:TYR:CE1	2.46	0.51
1:M:198:VAL:HB	1:M:207:VAL:HG12	1.93	0.51
1:U:184:VAL:CG2	1:U:185:PRO:HD2	2.41	0.51
1:A:2:VAL:HG13	1:A:102:TYR:CE1	2.45	0.51
2:K:197:THR:HG22	2:K:204:PRO:HB3	1.93	0.51
2:P:213:GLU:CG	2:P:214:CYS:N	2.74	0.51
2:R:197:THR:HG22	2:R: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:C	1:E:178:LEU:HD12	2.31	0.51
1:J:2:VAL:HG11	1:J:102:TYR:CZ	2.45	0.51
1:H:73:THR:HB	1:U:75:LYS:NZ	2.25	0.51
1:Q:143:LYS:HE2	1:Q:171:GLN:HE22	1.76	0.51
2:D:147:GLN:HG2	2:D:154:LEU:CD2	2.39	0.51
2:R:4:MET:O	2:R:5:THR:OG1	2.26	0.51
2:T:155:GLN:HE21	2:T:158:ASN:HD21	1.58	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
2:I:197:THR:HG22	2:I:204:PRO:HB3	1.93	0.50
1:S:214:LYS:CG	1:S:215:SER:N	2.74	0.50
1:C:82:MET:CE	1:C:82(C):LEU:HD11	2.41	0.50
1:C:216:CYS:O	1:C:217:ASP:CB	2.59	0.50
2:D:175:LEU:HD23	2:D:176:SER:N	2.26	0.50
1:O:143:LYS:HE2	1:O:171:GLN:HE22	1.76	0.50
2:P:112:ALA:HB1	2:P:201:LEU:CD1	2.40	0.50
1:U:188:SER:C	1:U:191:THR:HG23	2.28	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:C	1:U:178:LEU:HD12	2.32	0.50
2:N:29:VAL:HG23	2:N:66:ARG:HH21	1.76	0.50
1:C:178:LEU:HD12	1:C:178:LEU:C	2.32	0.50
1:H:56:TYR:CE1	1:U:18:LEU:HD13	2.46	0.50
1:H:198:VAL:HB	1:H:207:VAL:HG12	1.94	0.50
1:U:184:VAL:HG11	1:U:194:TYR:CZ	2.45	0.50
1:M:82:MET:CE	1:M:90:TYR:CZ	2.95	0.49
1:J:192:GLN:NE2	1:J:193:THR:H	2.10	0.49
2:X:212:GLY:C	2:X:214:CYS:H	2.15	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:F:197:THR:HG22	2:F:204:PRO:HB3	1.95	0.49
2:L:197:THR:HG22	2:L:204:PRO:HB3	1.93	0.49
2:F:24:ARG:HD3	2:V:157:GLY:HA2	1.95	0.49
2:R:112:ALA:HB1	2:R:201:LEU:CD1	2.43	0.49
2:X:197:THR:HG22	2:X:204:PRO:HB3	1.94	0.49
2:P:197:THR:HG22	2:P:204:PRO:HB3	1.95	0.49
2:X:24:ARG:NH2	4:X:301:NO3:O2	2.43	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:C:143:LYS:HE2	1:C:171:GLN:HE22	1.79	0.48
1:S:143:LYS:HE2	1:S:171:GLN:HE22	1.78	0.48
2:B:112:ALA:HB1	2:B:201:LEU:CD1	2.43	0.48
2:F:112:ALA:HB1	2:F:201:LEU:CD1	2.44	0.48
1:U:2:VAL:CG1	1:U:102:TYR:CZ	2.96	0.48
2:V:113:PRO:CD	2:V:198:HIS:ND1	2.77	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:HD23	2:D:175:LEU:C	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
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:L:189:HIS:O	2:L:211:ARG:NH2	2.46	0.47
2:V:113:PRO:CD	2:V:198:HIS:CE1	2.97	0.47
1:E:143:LYS:HE2	1:E:171:GLN:HE22	1.80	0.47
2:V:113:PRO:HG2	2:V:198:HIS:ND1	2.28	0.47
1:C:82:MET:HE2	1:C:82(C):LEU:HD11	1.96	0.47
2:I:18:ARG:HD3	2:R:153:ALA:HB2	1.97	0.47
1:M:193:THR:N	2:R:77:SER:OG	2.44	0.47
2:I:37:GLN:HB2	2:I:47:LEU:HD21	1.95	0.47
1:O:73:THR:CG2	1:S:156:SER:HB3	2.44	0.47
1:U:2:VAL:HG11	1:U:102:TYR:CE2	2.50	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:G:147:PRO:O	1:G:200:HIS:HE1	1.98	0.47
2:T:103:LYS:NZ	2:T:165:GLU:OE1	2.42	0.47
1:W:2:VAL:HG13	1:W:102:TYR:CE1	2.50	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: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:113:PRO:CG	2:V:198:HIS:CE1	2.98	0.46
2:V:199:GLN:HE21	2:V:199:GLN:HB3	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:H:147:PRO:O	1:H:200:HIS:HE1	1.99	0.46
1:M:82:MET:HE1	1:M:90:TYR:CZ	2.51	0.46
2:V:29:VAL:HG13	2:V:66:ARG:HH21	1.80	0.46
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.98	0.46
1:O:73:THR:CG2	1:S:156:SER:CB	2.93	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:M:147:PRO:O	1:M:200:HIS:HE1	1.98	0.45
1:U:147:PRO:O	1:U:200:HIS:HE1	1.99	0.45
2:L:153:ALA:HB2	2:X:18:ARG:HD3	1.96	0.45
1:A:147:PRO:O	1:A:200:HIS:HE1	1.99	0.45
2:K:12:SER:HB2	2:P:147:GLN:HE22	1.82	0.45
2:N:29:VAL:O	2:N:29:VAL:HG13	2.15	0.45
1:E:147:PRO:O	1:E:200:HIS:HE1	2.00	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: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
1:C:147:PRO:O	1:C:200:HIS:HE1	2.00	0.45
2:V:205:VAL:HG13	2:V:206:THR:N	2.30	0.45
2:R:4:MET:HG3	2:R:5:THR:HG23	1.99	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
1:O:82:MET:CE	1:O:82(C):LEU:HD11	2.46	0.45
2:I:163:VAL:HG22	2:I:175:LEU:HD12	1.97	0.45
1:O:147:PRO:O	1:O:200:HIS:HE1	2.00	0.44
2:P:151:ASP:O	2:P:152:ASN:CG	2.55	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:J:2:VAL:HG13	1:J:102:TYR:CE1	2.52	0.44
1:S:156:SER:N	1:S:197:ASN:HD21	2.03	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:O:178:LEU:HD12	1:O:178:LEU:C	2.37	0.44
1:Q:147:PRO:O	1:Q:200:HIS:HE1	2.00	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:D:18:ARG:HD3	2:N:153:ALA:HB2	1.98	0.44
2:F:78:LEU:CD2	2:F:82:ASP:HB2	2.48	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:C:67:PHE:CZ	1:C:82:MET:HE3	2.54	0.43
1:S:214:LYS:HE2	1:S:214:LYS:HB2	1.72	0.43
1:U:184:VAL:CB	1:U:185:PRO:CD	2.96	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:N:27:GLN:HB2	2:N:90:GLN:HG3	2.00	0.43
2:X:103:LYS:NZ	2:X:165:GLU:OE1	2.41	0.43
2:X:120:PRO:HD3	2:X:132:VAL:HG22	2.01	0.43
1:C:82:MET:HB3	1:C:82(C):LEU:HD11	1.99	0.43
2:D:155:GLN:NE2	2:D:158:ASN:HD21	2.09	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
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
2:V:108:ARG:CD	2:V:170:ASP:O	2.67	0.43
2:K:27:GLN:HB2	2:K:90:GLN:HG3	2.01	0.43
2:R:27:GLN:HB2	2:R:90:GLN:HG3	2.00	0.43
2:R:175:LEU:HD23	2:R:176:SER:N	2.34	0.43
1:U:143:LYS:HE2	1:U:171:GLN:HE22	1.84	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
2:B:27:GLN:HB2	2:B:90:GLN:HG3	2.01	0.42
2:F:120:PRO:HD3	2:F:132:VAL:HG22	2.02	0.42
2:L:120:PRO:HD3	2:L:132:VAL:HG22	2.01	0.42
1:C:166:PHE:CE2	2:D:176:SER:HB3	2.54	0.42
2:R:209:PHE:C	2:R:210:ASN:HD22	2.23	0.42
1:E:56:TYR:CD1	1:W:18:LEU:HD13	2.54	0.42
1:M:166:PHE:CE1	2:N:164:THR:HG23	2.54	0.42
2:R:175:LEU:HD23	2:R:175:LEU:C	2.39	0.42
1:H:73:THR:HB	1:U:75:LYS:HZ3	1.84	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
2:I:24:ARG:NH2	4:I:301:NO3:O1	2.53	0.42
2:I:120:PRO:HD3	2:I:132:VAL:HG22	2.00	0.42
1:U:185:PRO:O	1:U:186:SER:C	2.57	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:C:43:LYS:HE3	2:D:7:SER:OG	2.20	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
2:F:146:VAL:CG1	2:F:147:GLN:N	2.82	0.41
2:R:45:LYS:CE	2:R:45:LYS:HA	2.49	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
1:U:185:PRO:HG2	1:U:185:PRO:O	2.20	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:C:28:ASN:HD22	1:C:29:VAL:N	2.18	0.41
2:F:78:LEU:HD13	2:F:83:PHE:CZ	2.56	0.41
1:M:191:THR:O	2:R:77:SER:HB3	2.20	0.41
1:U:188:SER:HA	1:U:191:THR:CG2	2.49	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: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
1:W:82:MET:HB3	1:W:82(C):LEU:HD11	2.03	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
2:T:120:PRO:HD3	2:T:132:VAL:HG22	2.02	0.41
1:U:4:LEU:HD21	1:U:27:PHE:CZ	2.56	0.41
1:J:2:VAL:HG11	1:J:102:TYR:CE2	2.56	0.40
2:K:210:ASN:N	2:K:210:ASN:ND2	2.68	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:D:210:ASN:N	2:D:210:ASN:ND2	2.67	0.40
2:F:210:ASN:N	2:F:210:ASN:ND2	2.68	0.40
2:X:175:LEU:HD23	2:X:175:LEU:C	2.42	0.40
2:R:44:PRO:O	2:R:45:LYS:HE2	2.22	0.40
2:R:112:ALA:HB1	2:R:201:LEU:HD13	2.03	0.40
2:X:210:ASN:N	2:X:210:ASN:ND2	2.68	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	29	48
1	H	215/229 (94%)	213 (99%)	2 (1%)	0	100	100
1	J	222/229 (97%)	220 (99%)	1 (0%)	1 (0%)	29	48
1	M	216/229 (94%)	215 (100%)	0	1 (0%)	29	48
1	O	221/229 (96%)	218 (99%)	2 (1%)	1 (0%)	29	48
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%)	29	48
1	W	214/229 (93%)	212 (99%)	1 (0%)	1 (0%)	29	48
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%)	29	48
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%)	15	28
2	X	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	29	48
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%)	47	68

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 (i)

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%)	27	51
1	C	179/189 (95%)	170 (95%)	9 (5%)	24	46
1	E	173/189 (92%)	168 (97%)	5 (3%)	42	69
1	G	178/189 (94%)	169 (95%)	9 (5%)	24	45
1	H	179/189 (95%)	173 (97%)	6 (3%)	37	63
1	J	182/189 (96%)	175 (96%)	7 (4%)	33	58
1	M	181/189 (96%)	175 (97%)	6 (3%)	38	64
1	O	183/189 (97%)	175 (96%)	8 (4%)	28	52
1	Q	177/189 (94%)	172 (97%)	5 (3%)	43	70
1	S	177/189 (94%)	168 (95%)	9 (5%)	24	45
1	U	177/189 (94%)	165 (93%)	12 (7%)	16	30
1	W	178/189 (94%)	172 (97%)	6 (3%)	37	63
2	B	185/190 (97%)	171 (92%)	14 (8%)	13	25
2	D	185/190 (97%)	176 (95%)	9 (5%)	25	47
2	F	182/190 (96%)	171 (94%)	11 (6%)	19	37
2	I	185/190 (97%)	175 (95%)	10 (5%)	22	42
2	K	185/190 (97%)	174 (94%)	11 (6%)	19	37
2	L	184/190 (97%)	174 (95%)	10 (5%)	22	42
2	N	185/190 (97%)	174 (94%)	11 (6%)	19	37
2	P	185/190 (97%)	173 (94%)	12 (6%)	17	33
2	R	186/190 (98%)	175 (94%)	11 (6%)	19	37
2	T	185/190 (97%)	174 (94%)	11 (6%)	19	37
2	V	185/190 (97%)	168 (91%)	17 (9%)	9	18
2	X	185/190 (97%)	174 (94%)	11 (6%)	19	37
3	a	12/18 (67%)	11 (92%)	1 (8%)	11	22
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%)	13	25
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%)	2 4
3	m	13/18 (72%)	11 (85%)	2 (15%)	2 5
3	o	12/18 (67%)	8 (67%)	4 (33%)	0 0
3	q	18/18 (100%)	15 (83%)	3 (17%)	2 4
3	s	12/18 (67%)	10 (83%)	2 (17%)	2 4
3	u	13/18 (72%)	10 (77%)	3 (23%)	1 1
3	w	12/18 (67%)	11 (92%)	1 (8%)	11 22
All	All	4522/4764 (95%)	4274 (94%)	248 (6%)	21 41

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

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	I	301	-	1,3,3	0.31	0	0,3,3	-	-
4	NO3	B	301	-	1,3,3	0.28	0	0,3,3	-	-
4	NO3	N	302	-	1,3,3	0.41	0	0,3,3	-	-
4	NO3	T	301	-	1,3,3	0.42	0	0,3,3	-	-
5	EDO	W	301	-	3,3,3	0.31	0	2,2,2	0.52	0
4	NO3	P	301	-	1,3,3	0.25	0	0,3,3	-	-
4	NO3	K	301	-	1,3,3	0.43	0	0,3,3	-	-
4	NO3	D	301	-	1,3,3	0.26	0	0,3,3	-	-
4	NO3	R	301	-	1,3,3	0.34	0	0,3,3	-	-
5	EDO	Q	301	-	3,3,3	0.45	0	2,2,2	0.15	0
4	NO3	X	301	-	1,3,3	0.32	0	0,3,3	-	-
5	EDO	N	301	-	3,3,3	0.54	0	2,2,2	0.10	0
4	NO3	F	301	-	1,3,3	0.34	0	0,3,3	-	-
4	NO3	L	301	-	1,3,3	0.22	0	0,3,3	-	-
4	NO3	V	301	-	1,3,3	0.29	0	0,3,3	-	-

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
5	EDO	N	301	-	-	1/1/1/1	-
5	EDO	Q	301	-	-	0/1/1/1	-
5	EDO	W	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	301	EDO	O1-C1-C2-O2
5	W	301	EDO	O1-C1-C2-O2

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^{th} 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^2)	Q<0.9
1	A	217/229 (94%)	0.09	0 100 100	30, 45, 74, 109	0
1	C	219/229 (95%)	0.11	2 (0%) 84 86	24, 36, 67, 108	0
1	E	212/229 (92%)	0.77	29 (13%) 3 2	38, 61, 111, 133	0
1	G	218/229 (95%)	0.12	5 (2%) 60 63	29, 39, 59, 122	0
1	H	219/229 (95%)	0.10	1 (0%) 91 91	25, 36, 62, 81	0
1	J	224/229 (97%)	0.33	8 (3%) 42 46	27, 46, 90, 110	0
1	M	220/229 (96%)	0.10	4 (1%) 68 71	24, 36, 59, 109	0
1	O	223/229 (97%)	0.23	5 (2%) 62 65	36, 47, 76, 108	0
1	Q	217/229 (94%)	0.14	4 (1%) 68 71	24, 40, 75, 101	0
1	S	215/229 (93%)	0.27	9 (4%) 36 39	30, 49, 91, 113	0
1	U	217/229 (94%)	0.89	43 (19%) 1 1	34, 52, 125, 144	0
1	W	218/229 (95%)	0.17	3 (1%) 75 77	31, 44, 63, 118	0
2	B	210/215 (97%)	0.26	4 (1%) 66 69	42, 56, 73, 101	0
2	D	210/215 (97%)	0.16	4 (1%) 66 69	30, 42, 61, 101	0
2	F	207/215 (96%)	0.80	23 (11%) 5 5	45, 71, 97, 107	0
2	I	211/215 (98%)	0.17	5 (2%) 59 62	31, 42, 63, 104	0
2	K	210/215 (97%)	0.28	1 (0%) 91 91	29, 48, 72, 97	0
2	L	209/215 (97%)	0.17	3 (1%) 75 77	31, 43, 61, 93	0
2	N	210/215 (97%)	0.19	2 (0%) 82 84	30, 41, 60, 90	0
2	P	210/215 (97%)	0.31	6 (2%) 51 55	32, 50, 74, 90	0
2	R	211/215 (98%)	0.13	4 (1%) 66 69	25, 39, 61, 107	0
2	T	210/215 (97%)	0.53	14 (6%) 17 18	38, 59, 82, 111	0
2	V	210/215 (97%)	0.93	26 (12%) 4 3	50, 68, 99, 114	0
2	X	210/215 (97%)	0.18	4 (1%) 66 69	33, 45, 68, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	a	12/19 (63%)	1.55	5 (41%) 0 0	64, 75, 88, 94	0
3	c	16/19 (84%)	1.32	3 (18%) 1 1	57, 75, 101, 107	0
3	e	13/19 (68%)	0.79	0 100 100	57, 68, 85, 90	0
3	g	13/19 (68%)	1.05	1 (7%) 13 13	60, 71, 88, 93	0
3	h	12/19 (63%)	2.00	6 (50%) 0 0	77, 87, 97, 99	0
3	j	19/19 (100%)	0.99	3 (15%) 2 1	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%)	0.85	2 (10%) 6 6	42, 53, 79, 80	0
3	s	12/19 (63%)	0.63	1 (8%) 11 11	51, 65, 86, 86	0
3	u	13/19 (68%)	1.38	2 (15%) 2 1	76, 84, 99, 124	0
3	w	12/19 (63%)	0.92	1 (8%) 11 11	72, 83, 95, 105	0
All	All	5303/5556 (95%)	0.33	238 (4%) 33 36	24, 46, 88, 144	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	136	ALA	10.9
1	S	215	SER	7.7
1	J	-1	ILE	7.5
1	U	161	SER	7.4
2	V	214	CYS	6.6
1	J	191	THR	6.4
2	V	5	THR	6.4
2	I	212	GLY	6.3
1	U	194	TYR	6.2
1	G	133	GLY	6.0
1	U	135	THR	5.8
1	U	137	ALA	5.8
2	F	192	TYR	5.7
1	U	154	TRP	5.6
1	O	0	SER	5.5
1	U	138	LEU	5.4
1	U	162	GLY	5.4
2	X	5	THR	5.3
2	P	214	CYS	5.2
1	G	216	CYS	5.1
1	J	132	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	U	133	GLY	5.0
1	E	136	ALA	4.9
1	E	135	THR	4.8
2	N	5	THR	4.8
1	M	0	SER	4.7
1	E	121	VAL	4.7
2	B	5	THR	4.7
1	W	216	CYS	4.7
3	u	13	ASN	4.6
1	W	0	SER	4.6
1	U	191	THR	4.4
1	U	215	SER	4.4
1	U	125	ALA	4.4
2	V	142	ARG	4.3
2	K	5	THR	4.3
1	E	124	LEU	4.3
2	R	30	SER	4.3
2	B	29	VAL	4.3
2	L	29	VAL	4.2
2	T	193	ALA	4.1
1	E	125	ALA	4.0
1	Q	217	ASP	4.0
2	R	4	MET	4.0
1	O	132	SER	4.0
2	V	29	VAL	3.9
1	E	194	TYR	3.9
3	o	10	LEU	3.9
2	N	29	VAL	3.9
1	W	215	SER	3.8
1	E	185	PRO	3.8
1	E	190	GLY	3.8
2	F	190	LYS	3.7
2	P	29	VAL	3.7
3	q	14	ALA	3.7
1	E	189	LEU	3.7
1	U	152	VAL	3.7
1	O	216	CYS	3.6
1	U	184	VAL	3.6
1	U	158	ALA	3.6
1	U	183	THR	3.6
2	T	214	CYS	3.6
1	E	204	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	0	SER	3.6
1	Q	0	SER	3.6
1	U	206	LYS	3.6
2	L	5	THR	3.5
1	U	216	CYS	3.5
1	E	122	PHE	3.5
1	E	138	LEU	3.5
2	F	127	SER	3.5
3	a	7	ARG	3.5
2	D	5	THR	3.4
1	J	131	THR	3.4
2	V	106	ILE	3.4
1	E	206	LYS	3.4
2	F	5	THR	3.4
2	V	141	PRO	3.4
2	T	190	LYS	3.4
2	V	111	ALA	3.3
2	I	5	THR	3.3
1	E	191	THR	3.3
3	h	1	ASN	3.2
2	F	191	VAL	3.2
2	I	4	MET	3.2
2	F	116	PHE	3.2
1	U	182	VAL	3.2
1	U	0	SER	3.2
2	T	30	SER	3.2
1	U	198	VAL	3.2
2	X	214	CYS	3.1
2	V	140	TYR	3.1
3	j	17	HIS	3.1
1	U	193	THR	3.1
2	V	116	PHE	3.1
3	o	12	LEU	3.0
2	V	137	ASN	3.0
2	F	153	ALA	3.0
1	U	160	THR	3.0
2	F	205	VAL	2.9
2	V	110	VAL	2.9
1	U	134	GLY	2.9
2	V	14	SER	2.9
1	U	195	ILE	2.9
2	D	30	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	30	SER	2.9
2	R	29	VAL	2.9
2	F	150	VAL	2.9
1	E	195	ILE	2.9
3	h	7	ARG	2.8
1	U	212	GLU	2.8
1	S	211	VAL	2.8
1	J	190	GLY	2.8
1	E	0	SER	2.8
1	C	217	ASP	2.8
3	h	4	GLU	2.7
1	G	214	LYS	2.7
2	P	5	THR	2.7
2	T	202	SER	2.7
1	E	207	VAL	2.7
1	E	134	GLY	2.7
3	c	15	VAL	2.7
2	V	172	THR	2.7
2	V	202	SER	2.7
2	F	149	LYS	2.7
2	F	122	ASP	2.7
2	F	115	VAL	2.7
1	U	214	LYS	2.7
1	U	155	ASN	2.6
2	R	5	THR	2.6
2	T	153	ALA	2.6
1	E	157	GLY	2.6
2	F	197	THR	2.6
1	M	128	SER	2.6
2	X	213	GLU	2.6
1	O	206	LYS	2.5
2	V	78	LEU	2.5
1	Q	215	SER	2.5
2	V	13	ALA	2.5
3	a	1	ASN	2.5
2	F	206	THR	2.5
3	s	12	LEU	2.5
3	g	11	GLU	2.5
2	V	54	LEU	2.5
1	H	0	SER	2.5
2	P	30	SER	2.5
1	S	137	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	U	213	PRO	2.5
2	F	179	LEU	2.5
3	h	6	ASP	2.5
1	E	158	ALA	2.4
3	u	12	LEU	2.4
1	U	211	VAL	2.4
1	Q	134	GLY	2.4
1	G	215	SER	2.4
1	S	-1	ILE	2.4
3	c	13	ASN	2.4
3	q	12	LEU	2.4
1	J	29	VAL	2.4
1	U	210	LYS	2.4
1	U	159	LEU	2.4
2	V	104	VAL	2.4
3	j	18	ASN	2.4
1	J	209	LYS	2.4
1	M	217	ASP	2.4
2	T	205	VAL	2.4
1	E	188	SER	2.4
1	J	0	SER	2.4
2	B	212	GLY	2.3
2	T	201	LEU	2.3
1	U	208	ASP	2.3
1	S	210	LYS	2.3
1	S	191	THR	2.3
3	j	12	LEU	2.3
1	S	122	PHE	2.3
2	V	175	LEU	2.3
3	a	12	LEU	2.3
2	I	29	VAL	2.3
2	F	209	PHE	2.3
1	E	177	SER	2.3
2	D	29	VAL	2.3
2	T	112	ALA	2.3
3	h	5	LEU	2.3
2	B	76	SER	2.3
2	F	203	SER	2.3
2	T	212	GLY	2.3
1	M	1	GLU	2.3
2	D	214	CYS	2.3
2	T	152	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	h	12	LEU	2.2
1	E	196	CYS	2.2
2	V	139	PHE	2.2
1	S	141	LEU	2.2
3	a	8	LEU	2.2
2	F	189	HIS	2.2
1	U	189	LEU	2.2
2	F	154	LEU	2.2
2	T	126	LYS	2.2
3	c	12	LEU	2.2
2	V	83	PHE	2.2
1	C	161	SER	2.2
1	E	198	VAL	2.2
1	U	207	VAL	2.2
3	o	1	ASN	2.2
3	a	10	LEU	2.2
2	F	126	LYS	2.1
2	V	138	ASN	2.1
2	F	200	GLY	2.1
3	o	7	ARG	2.1
2	I	106	ILE	2.1
3	o	4	GLU	2.1
1	U	164	HIS	2.1
2	V	144	ALA	2.1
1	E	175	LEU	2.1
1	U	157	GLY	2.1
2	T	5	THR	2.1
1	E	187	SER	2.1
2	P	68	GLY	2.1
1	E	142	VAL	2.1
1	U	192	GLN	2.1
2	F	155	GLN	2.1
1	E	123	PRO	2.1
1	S	189	LEU	2.1
1	U	199	ASN	2.1
2	V	6	GLN	2.1
2	X	29	VAL	2.1
2	P	78	LEU	2.1
2	V	114	SER	2.1
1	E	184	VAL	2.1
2	V	146	VAL	2.1
1	U	185	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	U	197	ASN	2.0
3	w	1	ASN	2.0
1	U	127	SER	2.0
1	U	153	SER	2.0
1	O	217	ASP	2.0
2	T	184	ALA	2.0
2	F	207	LYS	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 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^{th} 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^2)	Q<0.9
5	EDO	W	301	4/4	0.73	0.24	47,47,48,48	0
4	NO3	V	301	4/4	0.79	0.62	37,39,39,39	4
4	NO3	B	301	4/4	0.84	0.30	59,59,63,66	0
4	NO3	L	301	4/4	0.87	0.29	26,26,27,27	4
5	EDO	N	301	4/4	0.91	0.16	38,39,39,40	0
4	NO3	I	301	4/4	0.92	0.20	49,49,52,55	0
4	NO3	F	301	4/4	0.92	0.33	26,26,27,28	4
4	NO3	P	301	4/4	0.92	0.31	30,31,31,32	4
5	EDO	Q	301	4/4	0.95	0.26	32,33,33,33	0
4	NO3	K	301	4/4	0.95	0.31	41,42,42,47	0
4	NO3	X	301	4/4	0.96	0.16	47,49,49,50	0
4	NO3	T	301	4/4	0.97	0.30	22,23,23,23	4
4	NO3	D	301	4/4	0.97	0.27	41,45,45,47	0
4	NO3	N	302	4/4	0.98	0.14	41,42,43,45	0
4	NO3	R	301	4/4	0.99	0.20	38,38,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.