



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:28 AM UTC

PDB ID : 4XGZ / pdb_00004xgz
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

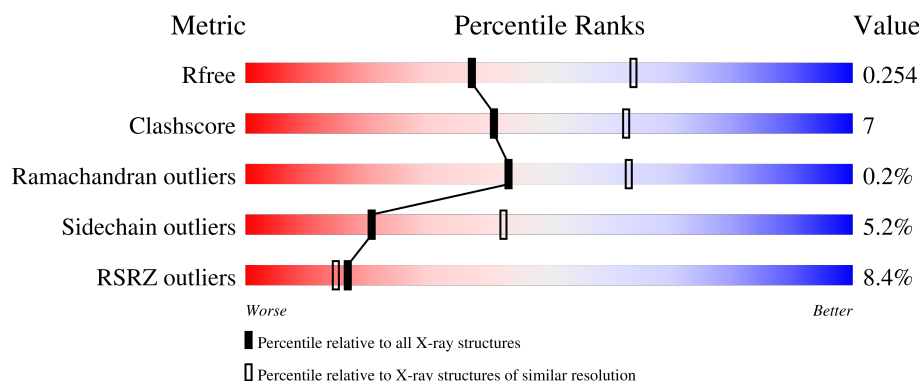
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	3% 86% 8% 5%
1	C	229	2% 84% 11% • •
1	E	229	21% 83% 9% 7%
1	G	229	3% 86% 7% • 5%
1	H	229	• 84% 10% •

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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	11%37%26%5%32%
3	o	19	42%26%21%16%37%
3	q	19	5%53%37%11%
3	s	19	11%26%32%5%37%
3	u	19	32%37%16%16%32%
3	w	19	21%37%26%37%

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.

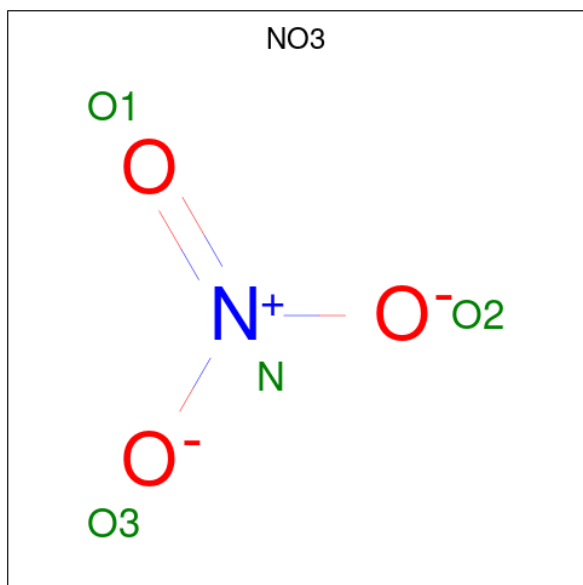
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	a	12	Total	C	N	O	0	0	0
			99	63	16	20			
3	c	16	Total	C	N	O	0	0	0
			128	80	22	26			
3	e	13	Total	C	N	O	0	0	0
			107	67	18	22			
3	g	13	Total	C	N	O	0	0	0
			107	67	18	22			
3	h	12	Total	C	N	O	0	0	0
			99	63	16	20			
3	j	19	Total	C	N	O	0	0	0
			153	95	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 (CCD ID: NO3) (formula: NO₃).



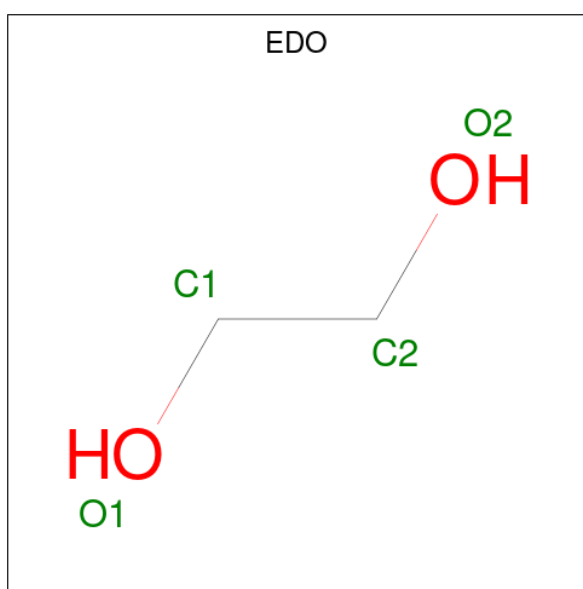
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	N	O	0	0
			4	1	3		
4	D	1	Total	N	O	0	0
			4	1	3		
4	F	1	Total	N	O	0	0
			4	1	3		
4	I	1	Total	N	O	0	0
			4	1	3		
4	K	1	Total	N	O	0	0
			4	1	3		
4	L	1	Total	N	O	0	0
			4	1	3		
4	N	1	Total	N	O	0	0
			4	1	3		
4	P	1	Total	N	O	0	0
			4	1	3		

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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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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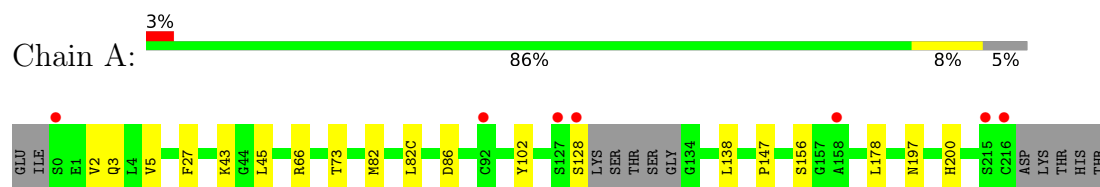
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	X	12	Total 12	O 12	0	0
6	a	1	Total 1	O 1	0	0
6	c	1	Total 1	O 1	0	0
6	e	1	Total 1	O 1	0	0
6	g	2	Total 2	O 2	0	0
6	j	4	Total 4	O 4	0	0
6	m	1	Total 1	O 1	0	0
6	o	1	Total 1	O 1	0	0
6	q	3	Total 3	O 3	0	0
6	s	1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

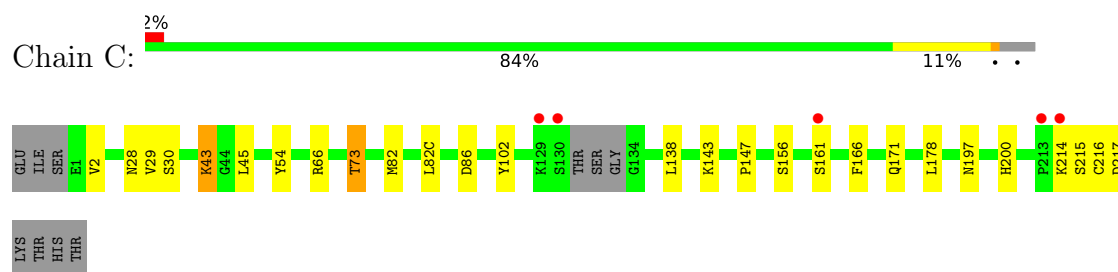
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

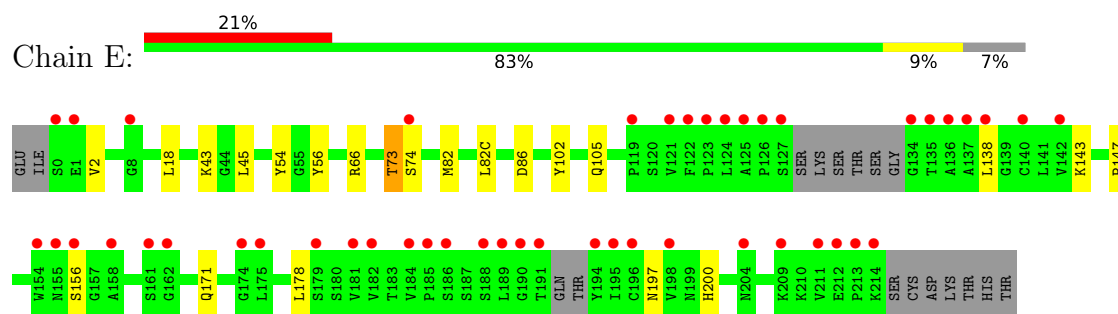
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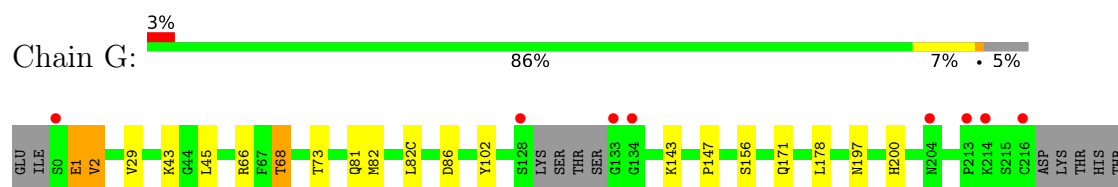
• Molecule 1: FAB HEAVY CHAIN



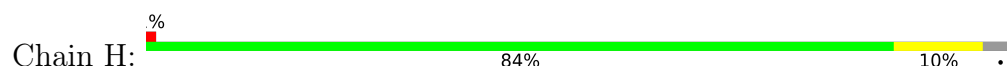
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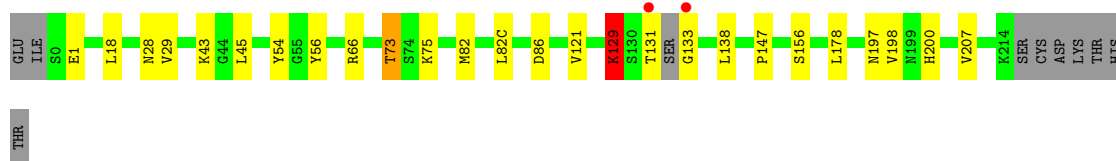


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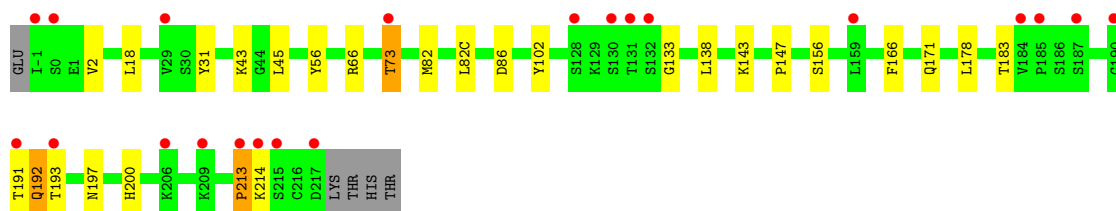
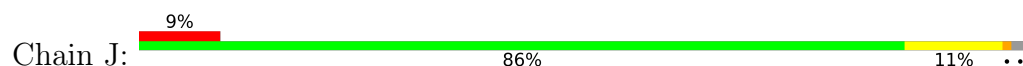


• Molecule 1: FAB HEAVY CHAIN

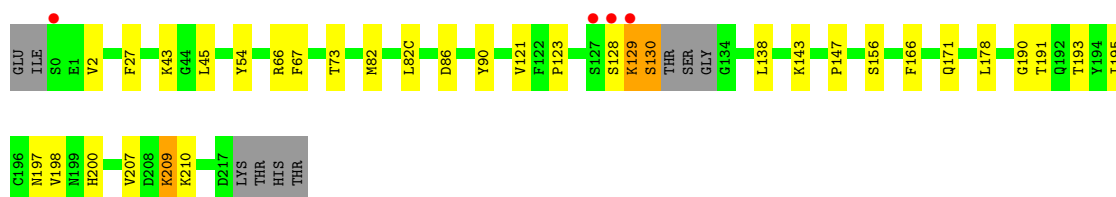
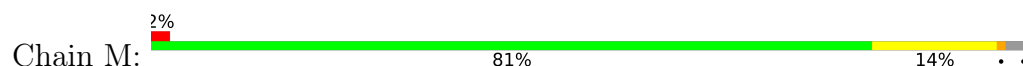




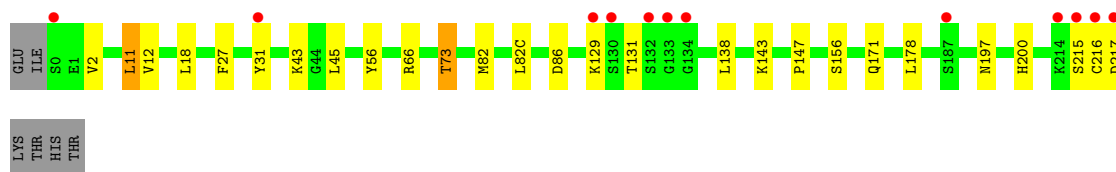
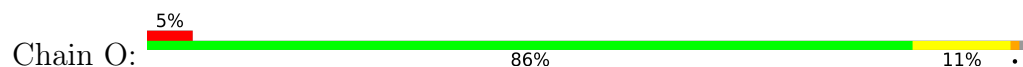
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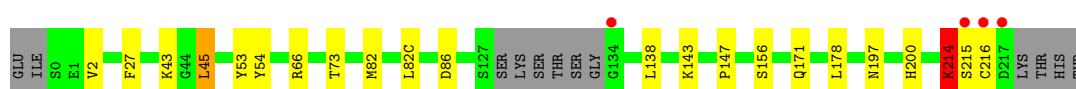
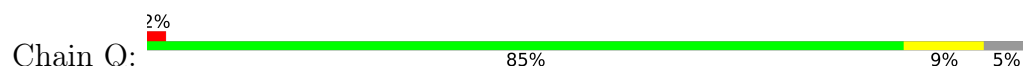
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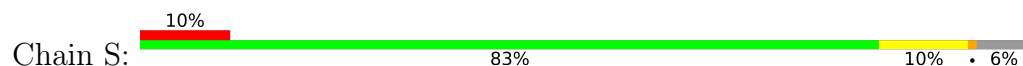
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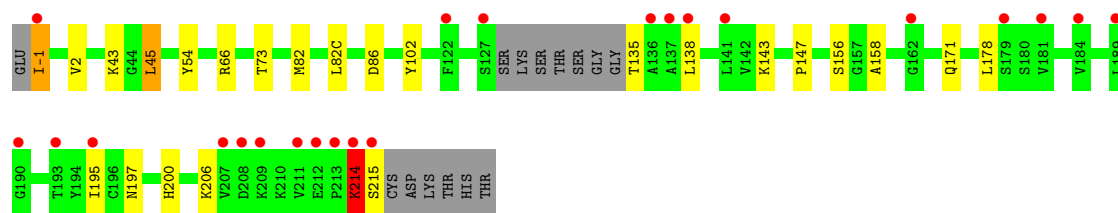


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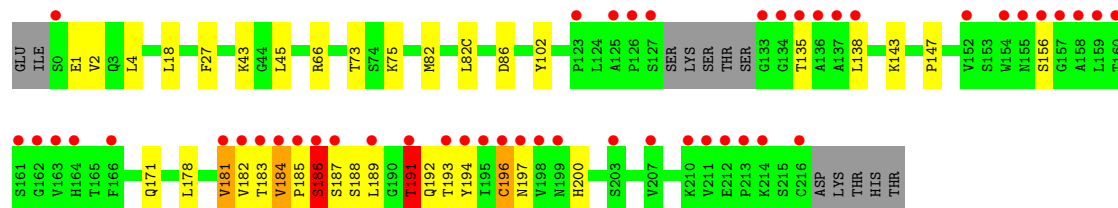


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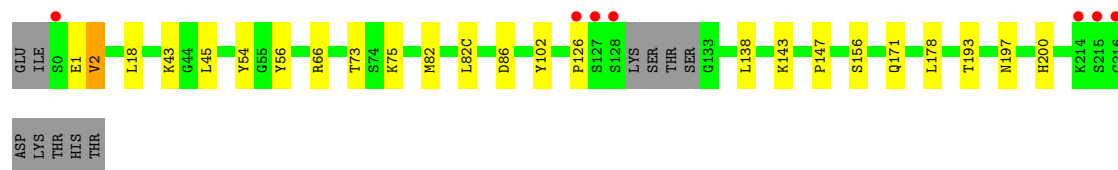
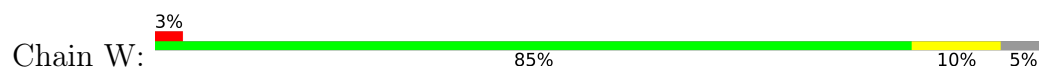




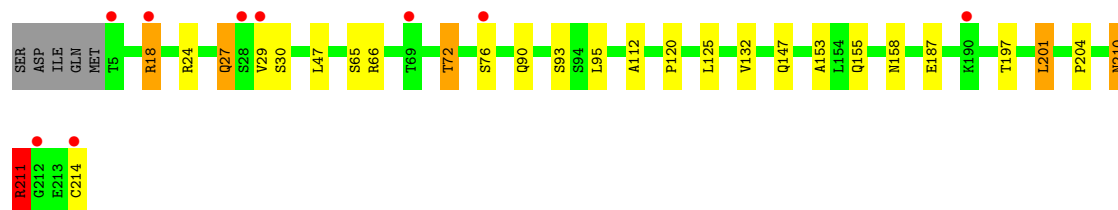
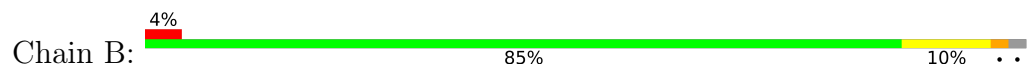
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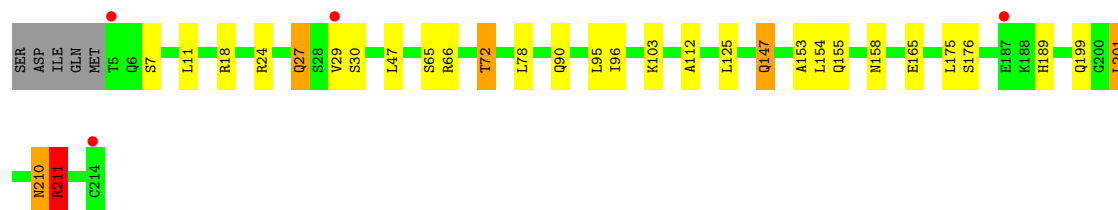
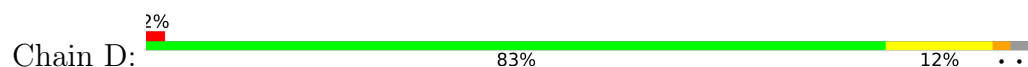
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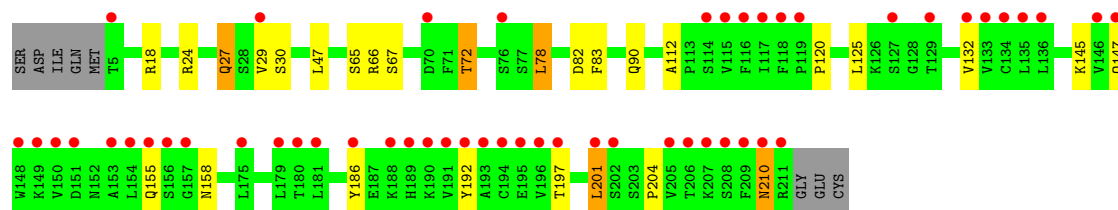
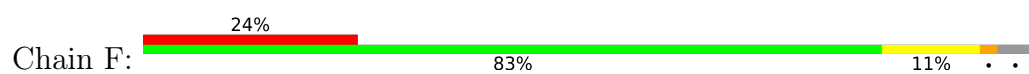
• Molecule 2: FAB LIGHT CHAIN



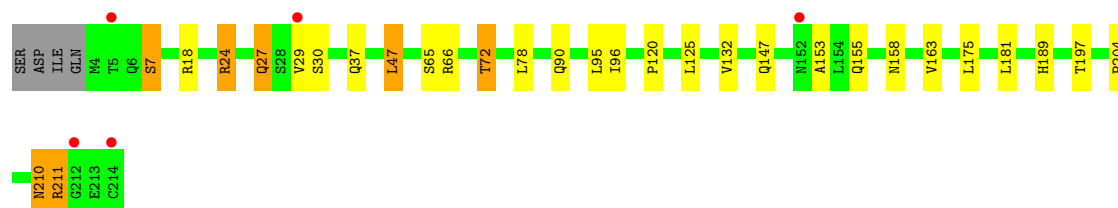
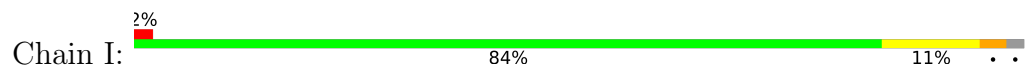
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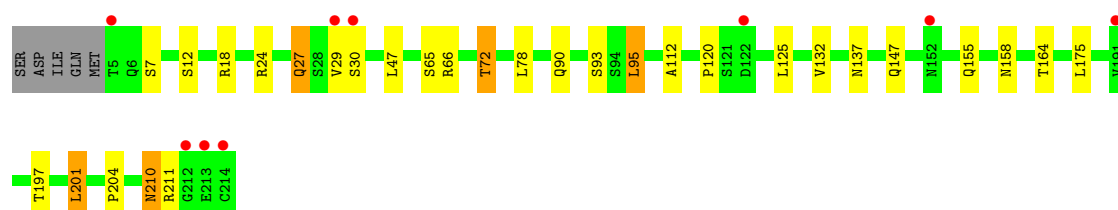
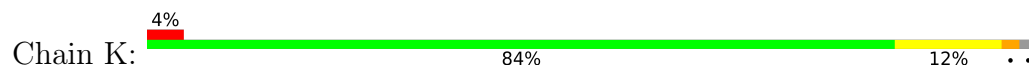
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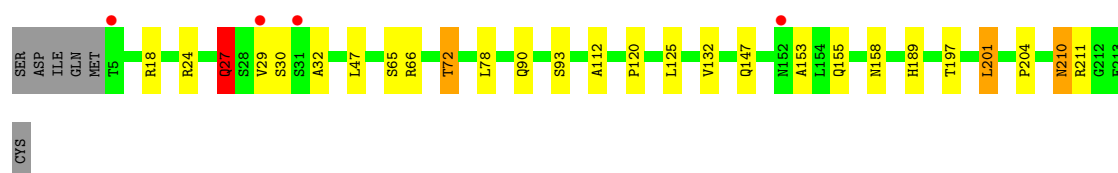
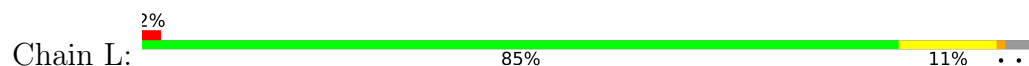
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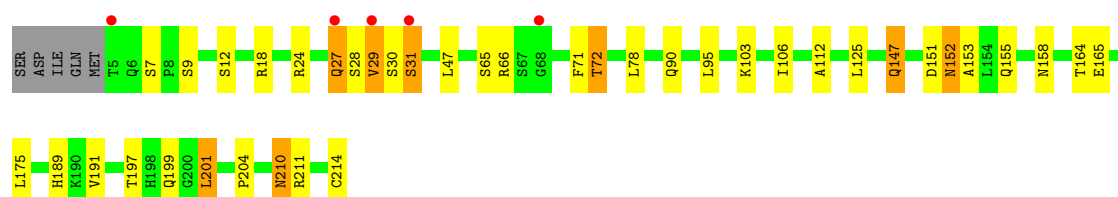
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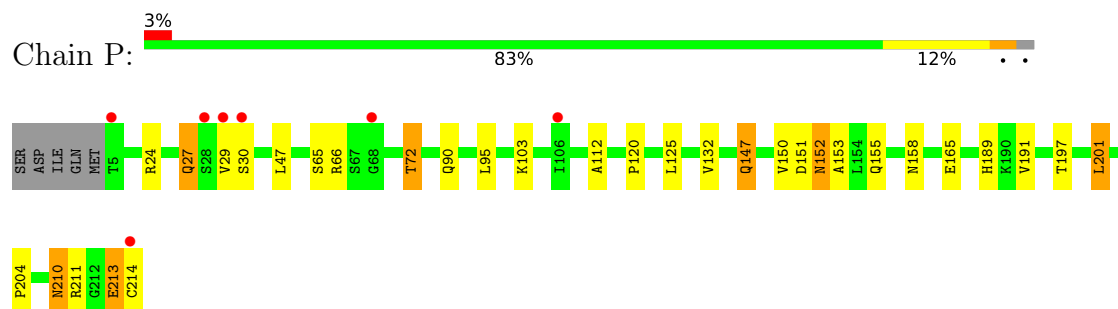
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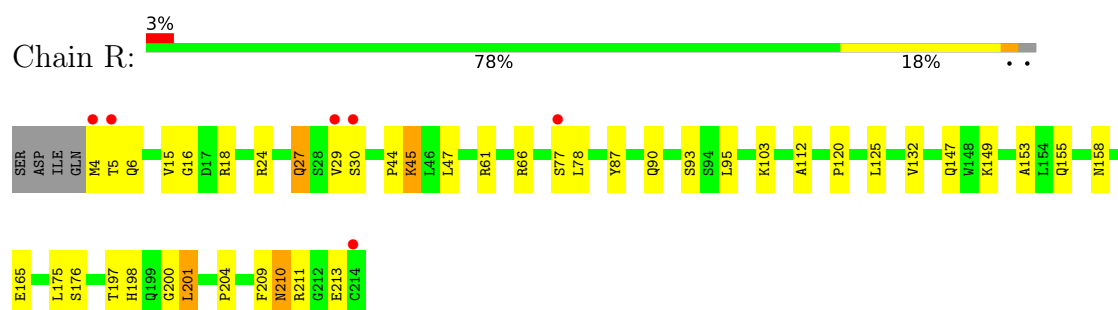
• Molecule 2: FAB LIGHT CHAIN



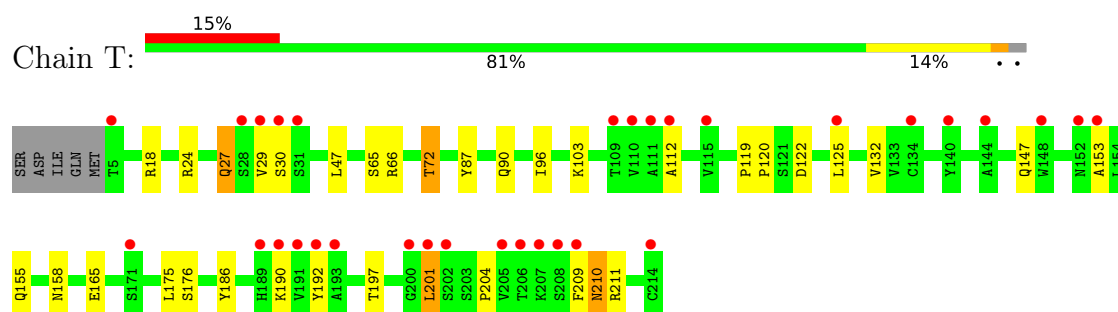
● Molecule 2: FAB LIGHT CHAIN



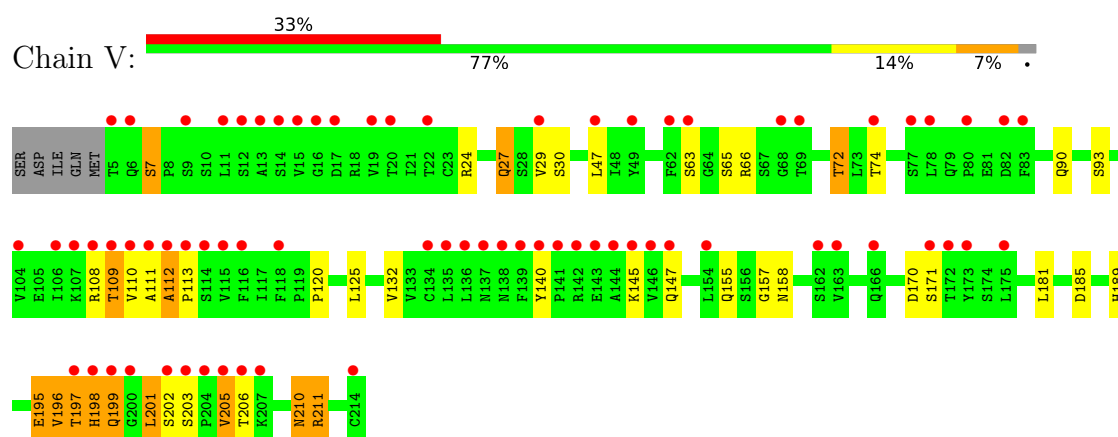
● Molecule 2: FAB LIGHT CHAIN



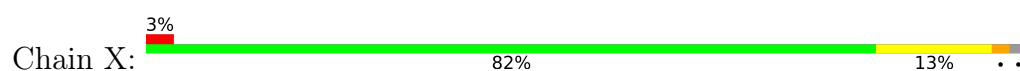
● Molecule 2: FAB LIGHT CHAIN

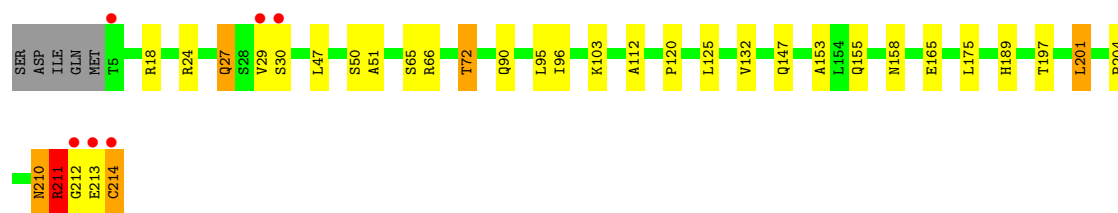


● Molecule 2: FAB LIGHT CHAIN

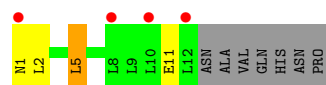


● Molecule 2: FAB LIGHT CHAIN





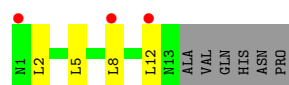
● Molecule 3: PAXILLIN LD2



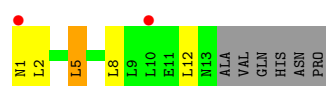
● Molecule 3: PAXILLIN LD2



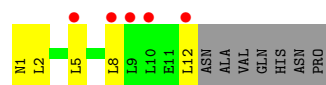
● Molecule 3: PAXILLIN LD2



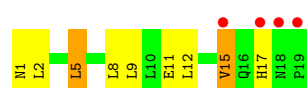
● Molecule 3: PAXILLIN LD2



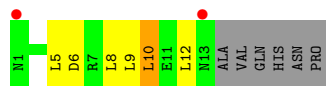
● Molecule 3: PAXILLIN LD2



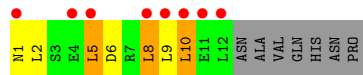
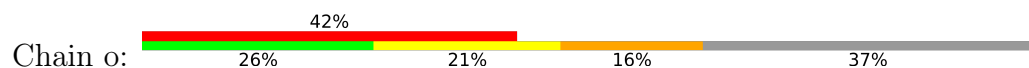
● Molecule 3: PAXILLIN LD2



- Molecule 3: PAXILLIN LD2



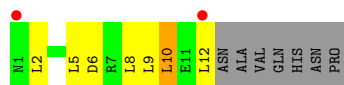
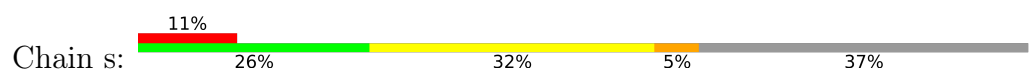
- Molecule 3: PAXILLIN LD2



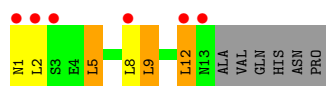
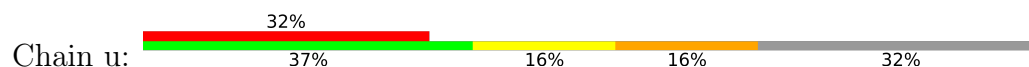
- Molecule 3: PAXILLIN LD2



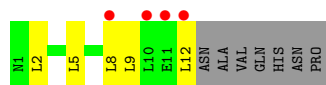
- Molecule 3: PAXILLIN LD2



- 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, α , β , γ	108.19Å 111.00Å 143.87Å 94.65° 95.28° 114.53°	Depositor
Resolution (Å)	142.00 – 2.50 142.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.3 (142.00-2.50) 94.2 (142.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ 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	9884 reflections (4.76%)	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 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/1661	0.64	0/2265
1	C	0.58	0/1674	0.66	0/2283
1	E	0.61	2/1626 (0.1%)	0.68	2/2216 (0.1%)
1	G	0.56	0/1665	0.65	0/2270
1	H	0.59	1/1675 (0.1%)	0.67	1/2283 (0.0%)
1	J	0.60	1/1704 (0.1%)	0.70	2/2325 (0.1%)
1	M	0.57	0/1684	0.67	0/2295
1	O	0.56	0/1702	0.66	1/2321 (0.0%)
1	Q	0.57	1/1659 (0.1%)	0.65	1/2264 (0.0%)
1	S	0.57	1/1653 (0.1%)	0.66	1/2255 (0.0%)
1	U	0.63	0/1659	0.82	4/2262 (0.2%)
1	W	0.57	0/1665	0.67	1/2270 (0.0%)
2	B	0.51	0/1625	0.68	1/2205 (0.0%)
2	D	0.54	0/1625	0.69	2/2205 (0.1%)
2	F	0.53	0/1600	0.65	0/2173
2	I	0.53	0/1630	0.71	3/2212 (0.1%)
2	K	0.51	0/1625	0.66	1/2205 (0.0%)
2	L	0.50	0/1619	0.67	1/2197 (0.0%)
2	N	0.56	0/1625	0.68	1/2205 (0.0%)
2	P	0.51	0/1625	0.67	0/2205
2	R	0.52	0/1633	0.72	3/2215 (0.1%)
2	T	0.55	1/1625 (0.1%)	0.69	1/2205 (0.0%)
2	V	0.63	0/1625	0.83	4/2205 (0.2%)
2	X	0.53	0/1625	0.69	1/2205 (0.0%)
3	a	0.87	0/98	1.17	2/131 (1.5%)
3	c	0.54	0/127	0.83	0/171
3	e	0.55	0/106	0.70	0/142
3	g	0.53	0/106	0.71	0/142
3	h	0.62	0/98	0.70	0/131
3	j	0.74	0/154	0.90	0/209
3	m	0.52	0/106	0.74	0/142
3	o	0.55	0/98	0.84	0/131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	q	0.75	0/154	0.89	0/209
3	s	0.60	0/98	0.71	0/131
3	u	0.64	0/106	1.00	0/142
3	w	0.52	0/98	0.71	0/131
All	All	0.56	7/40858 (0.0%)	0.69	33/55558 (0.1%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	105	GLN	C-O	8.21	1.33	1.24
1	E	105	GLN	CA-C	7.18	1.61	1.52
2	T	190	LYS	CA-CB	6.38	1.63	1.53
1	S	214	LYS	N-CA	-5.35	1.41	1.46
1	J	214	LYS	CA-C	5.33	1.59	1.52
1	H	1	GLU	CA-C	5.27	1.60	1.52
1	Q	214	LYS	N-CA	5.20	1.52	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	105	GLN	N-CA-C	-12.20	89.21	109.46
1	U	186	SER	N-CA-C	-11.45	98.80	111.28
1	U	196	CYS	CA-CB-SG	9.78	136.90	114.40
2	T	211	ARG	N-CA-C	9.56	122.90	111.33
1	S	214	LYS	N-CA-C	-9.51	96.30	111.04
2	R	211	ARG	N-CA-C	9.38	122.68	111.33
2	V	211	ARG	N-CA-C	9.09	122.33	111.33
2	B	211	ARG	N-CA-CB	8.83	123.01	109.85
1	W	126	PRO	N-CA-C	8.71	125.07	110.95
2	I	211	ARG	N-CA-C	8.60	125.56	111.37
2	D	211	ARG	CG-CD-NE	-7.59	95.31	112.00
3	a	11	GLU	CG-CD-OE2	-7.45	101.28	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	11	GLU	CG-CD-OE1	7.19	134.93	118.40
2	L	27	GLN	CA-CB-CG	7.04	128.18	114.10
2	V	196	VAL	CB-CA-C	-7.03	101.35	110.98
1	U	181	VAL	N-CA-C	6.88	118.03	108.12
2	I	211	ARG	CB-CA-C	-6.85	99.38	110.74
1	E	105	GLN	CA-C-O	6.66	128.07	120.54
2	V	7	SER	CB-CA-C	6.46	118.58	108.63
2	I	7	SER	CB-CA-C	6.39	118.47	108.63
1	U	191	THR	N-CA-C	6.28	117.92	111.14
2	N	31	SER	N-CA-CB	-6.04	104.77	113.65
1	H	129	LYS	N-CA-C	-6.02	103.06	110.65
1	Q	215	SER	N-CA-C	-5.86	106.27	113.41
2	D	211	ARG	N-CA-CB	5.85	118.56	109.85
2	V	205	VAL	CB-CA-C	-5.82	104.93	111.45
1	J	214	LYS	N-CA-C	5.77	118.15	107.99
2	K	211	ARG	NE-CZ-NH1	-5.38	116.12	121.50
2	X	211	ARG	N-CA-C	-5.33	99.45	110.80
1	O	215	SER	N-CA-C	5.23	117.39	111.11
2	R	211	ARG	NE-CZ-NH1	-5.21	116.29	121.50
2	R	6	GLN	N-CA-C	5.08	117.89	109.46
1	J	213	PRO	O-C-N	5.07	128.78	123.10

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	19	0
1	E	1586	0	1537	16	0
1	G	1624	0	1570	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1634	0	1586	24	0
1	J	1662	0	1600	21	1
1	M	1643	0	1589	34	0
1	O	1660	0	1605	17	0
1	Q	1618	0	1555	15	0
1	S	1612	0	1566	27	0
1	U	1618	0	1565	57	0
1	W	1624	0	1570	18	0
2	B	1593	0	1555	14	0
2	D	1593	0	1555	23	0
2	F	1568	0	1531	15	1
2	I	1598	0	1557	14	0
2	K	1593	0	1555	16	0
2	L	1587	0	1551	16	0
2	N	1593	0	1555	29	0
2	P	1593	0	1555	21	0
2	R	1601	0	1564	35	1
2	T	1593	0	1556	18	0
2	V	1593	0	1555	49	0
2	X	1593	0	1555	20	0
3	a	99	0	108	4	0
3	c	128	0	136	2	0
3	e	107	0	114	3	0
3	g	107	0	114	4	0
3	h	99	0	108	4	0
3	j	153	0	156	10	0
3	m	107	0	114	3	0
3	o	99	0	108	4	0
3	q	153	0	156	16	0
3	s	99	0	108	4	0
3	u	107	0	114	7	0
3	w	99	0	108	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	516	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 7.

All (516) 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
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
2:V:201:LEU:HD13	2:V:201:LEU:C	1.89	0.97
1:M:193:THR:HG22	2:R:77:SER:HG	1.31	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
1:U:185:PRO:CG	1:U:188:SER:HB2	2.01	0.90
3:u:1:ASN:O	3:u:5:LEU:HD13	1.70	0.90
2:N:28:SER:C	2:N:30:SER:H	1.82	0.87
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
1:C:82:MET:HE2	1:C:82(C):LEU:HD11	1.58	0.84
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	1.60	0.83
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
1:S:82:MET:HE2	1:S:82(C):LEU:HD11	1.59	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:108:ARG:NE	2:V:170:ASP:O	2.14	0.80
1:A:82:MET:HE2	1:A:82(C):LEU:HD11	1.62	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
1:C:30:SER:HB3	1:C:73:THR:HG22	1.63	0.78
1:O:82:MET:HE2	1:O:82(C):LEU:HD11	1.66	0.78
2:L:27:GLN:C	2:L:27:GLN:HE21	1.91	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: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
3:u:9:LEU:O	3:u:12:LEU:HD22	1.87	0.74
1:Q:156:SER:H	1:Q:197:ASN:HD21	1.34	0.74
3:u:8:LEU:O	3:u:12:LEU:HD13	1.87	0.74
1:Q:82:MET:HE2	1:Q:82(C):LEU:HD11	1.70	0.74
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
1:U:156:SER:H	1:U:197:ASN:HD21	1.35	0.72
1:J:82:MET:HE2	1:J:82(C):LEU:HD11	1.70	0.72
1:O:156:SER:H	1:O:197:ASN:HD21	1.37	0.72
2:V:201:LEU:C	2:V:201:LEU:CD1	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:o:1:ASN:O	3:o:5:LEU:HD13	1.91	0.71
1:W:82:MET:HE2	1:W:82(C):LEU:HD11	1.73	0.71
2:R:197:THR:HG23	6:R:403:HOH:O	1.90	0.71
3:a:1:ASN:O	3:a:5:LEU:HD13	1.91	0.71
1:C:156:SER:H	1:C:197:ASN:HD21	1.37	0.70
1:M:129:LYS:H	1:M:130:SER:C	2.00	0.70
2:V:195:GLU:O	2:V:195:GLU:CG	2.40	0.70
3:q:15:VAL:O	3:q:15:VAL:HG22	1.92	0.70
3:q:12:LEU:O	3:q:15:VAL:HG13	1.91	0.70
2:D:147:GLN:HG2	2:D:154:LEU:HD22	1.75	0.69
1:G:82:MET:HE2	1:G:82(C):LEU:HD11	1.74	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:M:82:MET:HE1	1:M:90:TYR:CZ	2.29	0.68
2:V:197:THR:OG1	2:V:198:HIS:N	2.21	0.67
3:j:15:VAL:HG22	3:j:15:VAL:O	1.94	0.67
2:D:211:ARG:NH1	2:D:211:ARG:HG2	2.10	0.67
2:N:28:SER:C	2:N:30:SER:N	2.44	0.67
2:V:63:SER:OG	2:V:74:THR:CG2	2.42	0.67
1:E:82:MET:HE2	1:E:82(C):LEU:HD11	1.75	0.66
2:I:153:ALA:HB2	2:R:18:ARG:HD3	1.76	0.66
2:R:93:SER:HA	3:q:1:ASN:H3	1.61	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:Q:53:TYR:CZ	3:q:12:LEU:HD21	2.29	0.66
1:U:82:MET:HE2	1:U:82(C):LEU:HD11	1.78	0.66
2:P:152:ASN:OD1	2:P:152:ASN:C	2.39	0.66
3:g:1:ASN:O	3:g:5:LEU:HD13	1.96	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
2:N:152:ASN:C	2:N:152:ASN:OD1	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:S:178:LEU:C	1:S:178:LEU:HD12	2.24	0.63
2:V:205:VAL:HG12	2:V:206:THR:N	2.12	0.63
2:B:93:SER:HA	3:a:1:ASN:H3	1.63	0.62
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
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: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
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:A:178:LEU:HD12	1:A:178:LEU:C	2.27	0.59
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:B:18:ARG:HD3	2:T:153:ALA:HB2	1.85	0.59
1:H:178:LEU:HD12	1:H:178:LEU:C	2.27	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
2:L:29:VAL:HG13	2:L:66:ARG:HH21	1.68	0.58
1:M:178:LEU:HD12	1:M:178:LEU:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:178:LEU:C	1:Q:178:LEU:HD12	2.29	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
1:M:129:LYS:N	1:M:130:SER:C	2.62	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
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
3:o:6:ASP:O	3:o:10:LEU:HD22	2.04	0.57
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
2:V:93:SER:HA	3:u:1:ASN:H3	1.70	0.56
3:j:12:LEU:O	3:j:15:VAL:HG13	2.06	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
2:L:93:SER:HA	3:h:1:ASN:H3	1.71	0.56
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:E:178:LEU:C	1:E:178:LEU:HD12	2.31	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
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
1:U:188:SER:C	1:U:191:THR:HG23	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:151:ASP:O	2:N:152:ASN:CG	2.50	0.55
1:U:66:ARG:NH2	1:U:86:ASP:OD2	2.40	0.55
1:U:178:LEU:C	1:U:178:LEU:HD12	2.32	0.55
1:W:2:VAL:HG11	1:W:102:TYR:CZ	2.42	0.55
1:C:178:LEU:HD12	1:C:178:LEU:C	2.32	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: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
2:X:212:GLY:C	2:X:214:CYS:H	2.15	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:W:54:TYR:CD2	3:w:5:LEU:HD22	2.42	0.54
3:a:2:LEU:HA	3:a:5:LEU:HD22	1.90	0.54
1:G:66:ARG:NH2	1:G:86:ASP:OD2	2.41	0.54
1:H:54:TYR:CD2	3:h:5:LEU:HD22	2.43	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
2:K:93:SER:HA	3:j:1:ASN:H3	1.73	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
1:E:54:TYR:CD2	3:e:5:LEU:HD22	2.43	0.53
2:L:27:GLN:HE21	2:L:27:GLN:CA	2.21	0.53
1:Q:53:TYR:CE2	3:q:12:LEU:HD21	2.42	0.53
1:U:2:VAL:HG11	1:U:102:TYR:CZ	2.44	0.53
3:o:2:LEU:HA	3:o:5:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:8:LEU:O	3:g:12:LEU:HD13	2.08	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
3:q:2:LEU:HA	3:q:5:LEU:HD22	1.91	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:M:54:TYR:CD2	3:m:5:LEU:HD22	2.44	0.53
1:O:31:TYR:CZ	1:S:206:LYS:NZ	2.77	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
3:g:2:LEU:HA	3:g:5:LEU:HD22	1.90	0.53
2:D:175:LEU:C	2:D:175:LEU:HD23	2.35	0.52
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
3:m:8:LEU:O	3:m:12:LEU:HD13	2.10	0.52
1:G:2:VAL:CG1	1:G:102:TYR:CZ	2.92	0.52
1:J:178:LEU:HD12	1:J:178:LEU:C	2.34	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
1:S:54:TYR:CD2	3:s:5:LEU:HD22	2.45	0.52
3:u:2:LEU:HA	3:u:5:LEU:HD22	1.90	0.52
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.91	0.52
1:C:54:TYR:CD2	3:c:5:LEU:HD22	2.45	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
3:m:6:ASP:O	3:m:10:LEU:HD13	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:103:LYS:NZ	2:D:165:GLU:OE1	2.40	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:R:197:THR:HG22	2:R:204:PRO:HB3	1.93	0.51
3:o:5:LEU:HA	3:o:8:LEU:HD22	1.93	0.51
1:J:2:VAL:HG11	1:J:102:TYR:CZ	2.45	0.51
3:h:8:LEU:O	3:h:12:LEU:HD13	2.10	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: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: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
2:D:189:HIS:O	2:D:211:ARG:NH1	2.43	0.50
2:N:29:VAL:HG23	2:N:66:ARG:HH21	1.76	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
3:e:8:LEU:O	3:e:12:LEU:HD13	2.12	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
1:Q:53:TYR:HB3	3:q:9:LEU:HD21	1.93	0.49
2:N:103:LYS:NZ	2:N:165:GLU:OE1	2.39	0.49
2:V:108:ARG:HG2	2:V:109:THR:N	2.26	0.49
3:h:2:LEU:HA	3:h:5:LEU:HD12	1.94	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:P:151:ASP:O	2:P:152:ASN:CG	2.55	0.49
3:e:2:LEU:HA	3:e:5:LEU:HD12	1.95	0.49
2:F:24:ARG:HD3	2:V:157:GLY:HA2	1.95	0.49
3:q:15:VAL:O	3:q:15:VAL:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:178:LEU:HD12	1:O:178:LEU:C	2.37	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
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
3:j:2:LEU:HA	3:j:5:LEU:HD22	1.94	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: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
2:L:189:HIS:O	2:L:211:ARG:NH2	2.46	0.47
1:U:188:SER:C	1:U:191:THR:CG2	2.87	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
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:R:209:PHE:C	2:R:210:ASN:HD22	2.23	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
2:R:175:LEU:C	2:R:175:LEU:HD23	2.39	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:U:185:PRO:O	1:U:186:SER:C	2.57	0.47
2:D:11:LEU:HD12	2:N:147:GLN:CD	2.40	0.47
1:G:147:PRO:O	1:G:200:HIS:HE1	1.98	0.47
2:T:96:ILE:HG13	3:s:2:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:u:8:LEU:O	3:u:12:LEU:CD1	2.60	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
2:P:150:VAL:HG12	2:P:155:GLN:CD	2.41	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
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
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
3:s:6:ASP:O	3:s:10:LEU:HD13	2.15	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
3:j:1:ASN:O	3:j:5:LEU:HD13	2.16	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:O:216:CYS:O	1:O:217:ASP:C	2.57	0.45
3:u:9:LEU:HA	3:u:12:LEU:HD21	1.99	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
2:X:175:LEU:HD23	2:X:175:LEU:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:163:VAL:HG22	2:I:175:LEU:HD12	1.97	0.45
2:D:96:ILE:HG13	3:c:2:LEU:HD21	1.99	0.44
1:O:147:PRO:O	1:O:200:HIS:HE1	2.00	0.44
2:X:210:ASN:C	2:X:212:GLY:N	2.75	0.44
3:q:2:LEU:HD12	3:q:2:LEU:O	2.16	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: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:W:178:LEU:C	1:W:178:LEU:HD12	2.43	0.44
3:q:1:ASN:O	3:q:5:LEU:HD13	2.17	0.44
2:R:103:LYS:NZ	2:R:165:GLU:OE1	2.41	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
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
3:w:8:LEU:O	3:w:12:LEU:HD13	2.17	0.43
1:G:178:LEU:C	1:G:178:LEU:HD12	2.43	0.43
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: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
3:j:11:GLU:OE2	3:q:17:HIS:HD2	2.02	0.43
2:I:96:ILE:HG13	3:g:2:LEU:HD21	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:93:SER:CA	3:a:1:ASN:H3	2.30	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
2:N:175:LEU:HD23	2:N:175:LEU:C	2.43	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
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
3:j:8:LEU:O	3:j:12:LEU:HD23	2.19	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:Q:53:TYR:CZ	3:q:12:LEU:CD2	3.00	0.42
1:Q:54:TYR:OH	3:q:8:LEU:HB3	2.20	0.42
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:R:45:LYS:CE	2:R:45:LYS:HA	2.49	0.41
1:M:82:MET:HE2	1:M:82(C):LEU:HD11	2.02	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
1:J:31:TYR:C	3:j:9:LEU:HD22	2.44	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
3:q:18:ASN:OD1	3:q:18:ASN:N	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:175:LEU:C	2:T:175:LEU:HD23	2.45	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
2:X:96:ILE:HG13	3:w:2:LEU:HD21	2.02	0.41
3:s:8:LEU:O	3:s:12:LEU:HD13	2.21	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
3:j:17:HIS:NE2	3:q:8:LEU:CD2	2.84	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:K:95:LEU:N	3:j:2:LEU:HD23	2.36	0.40
2:K:175:LEU:HD23	2:K:175:LEU:C	2.47	0.40
1:M:67:PHE:CE2	1:M:82:MET:HE3	2.56	0.40
1:Q:53:TYR:CB	3:q:9:LEU:HD21	2.52	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

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%)	24	43
1	H	215/229 (94%)	213 (99%)	2 (1%)	0	100	100
1	J	222/229 (97%)	220 (99%)	1 (0%)	1 (0%)	24	43
1	M	216/229 (94%)	215 (100%)	0	1 (0%)	24	43
1	O	221/229 (96%)	218 (99%)	2 (1%)	1 (0%)	24	43
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%)	24	43
1	W	214/229 (93%)	212 (99%)	1 (0%)	1 (0%)	24	43
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%)	24	43
2	P	208/215 (97%)	202 (97%)	6 (3%)	0	100	100
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%)	12	24
2	X	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	24	43
3	a	10/19 (53%)	10 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	43	63

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%)	172 (97%)	6 (3%)	32	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	179/189 (95%)	172 (96%)	7 (4%)	28	55
1	E	173/189 (92%)	169 (98%)	4 (2%)	44	72
1	G	178/189 (94%)	171 (96%)	7 (4%)	28	55
1	H	179/189 (95%)	174 (97%)	5 (3%)	38	66
1	J	182/189 (96%)	177 (97%)	5 (3%)	39	67
1	M	181/189 (96%)	174 (96%)	7 (4%)	28	55
1	O	183/189 (97%)	177 (97%)	6 (3%)	33	61
1	Q	177/189 (94%)	173 (98%)	4 (2%)	44	72
1	S	177/189 (94%)	170 (96%)	7 (4%)	28	54
1	U	177/189 (94%)	167 (94%)	10 (6%)	19	39
1	W	178/189 (94%)	173 (97%)	5 (3%)	38	66
2	B	185/190 (97%)	171 (92%)	14 (8%)	12	26
2	D	185/190 (97%)	173 (94%)	12 (6%)	15	32
2	F	182/190 (96%)	172 (94%)	10 (6%)	19	40
2	I	185/190 (97%)	173 (94%)	12 (6%)	15	32
2	K	185/190 (97%)	173 (94%)	12 (6%)	15	32
2	L	184/190 (97%)	174 (95%)	10 (5%)	20	41
2	N	185/190 (97%)	172 (93%)	13 (7%)	14	29
2	P	185/190 (97%)	173 (94%)	12 (6%)	15	32
2	R	186/190 (98%)	174 (94%)	12 (6%)	15	32
2	T	185/190 (97%)	176 (95%)	9 (5%)	22	45
2	V	185/190 (97%)	169 (91%)	16 (9%)	10	21
2	X	185/190 (97%)	174 (94%)	11 (6%)	18	37
3	a	12/18 (67%)	11 (92%)	1 (8%)	10	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%)	12	25
3	h	12/18 (67%)	12 (100%)	0	100	100
3	j	18/18 (100%)	16 (89%)	2 (11%)	6	12
3	m	13/18 (72%)	11 (85%)	2 (15%)	2	5
3	o	12/18 (67%)	8 (67%)	4 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	q	18/18 (100%)	16 (89%)	2 (11%)	6	12
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%)	10	22
All	All	4522/4764 (95%)	4288 (95%)	234 (5%)	21	42

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	43	LYS
1	A	45	LEU
1	A	73	THR
1	A	128	SER
1	A	138	LEU
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	95	LEU
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	43	LYS
1	C	45	LEU
1	C	73	THR
1	C	138	LEU
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

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Mol	Chain	Res	Type
2	D	78	LEU
2	D	95	LEU
2	D	125	LEU
2	D	147	GLN
2	D	201	LEU
2	D	210	ASN
2	D	211	ARG
1	E	43	LYS
1	E	45	LEU
1	E	73	THR
1	E	138	LEU
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	2	VAL
1	G	29	VAL
1	G	43	LYS
1	G	45	LEU
1	G	68	THR
1	G	73	THR
1	H	43	LYS
1	H	45	LEU
1	H	73	THR
1	H	129	LYS
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	78	LEU
2	I	95	LEU
2	I	125	LEU

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Mol	Chain	Res	Type
2	I	147	GLN
2	I	181	LEU
2	I	210	ASN
1	J	43	LYS
1	J	45	LEU
1	J	73	THR
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	78	LEU
2	K	95	LEU
2	K	125	LEU
2	K	147	GLN
2	K	201	LEU
2	K	210	ASN
2	L	24	ARG
2	L	27	GLN
2	L	30	SER
2	L	47	LEU
2	L	72	THR
2	L	78	LEU
2	L	125	LEU
2	L	147	GLN
2	L	201	LEU
2	L	210	ASN
1	M	43	LYS
1	M	45	LEU
1	M	73	THR
1	M	129	LYS
1	M	130	SER
1	M	138	LEU
1	M	209	LYS
2	N	7	SER
2	N	24	ARG
2	N	27	GLN
2	N	47	LEU
2	N	72	THR

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Mol	Chain	Res	Type
2	N	78	LEU
2	N	95	LEU
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	43	LYS
1	O	45	LEU
1	O	73	THR
1	O	129	LYS
1	O	138	LEU
2	P	24	ARG
2	P	27	GLN
2	P	30	SER
2	P	47	LEU
2	P	72	THR
2	P	95	LEU
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	43	LYS
1	Q	45	LEU
1	Q	73	THR
1	Q	138	LEU
2	R	24	ARG
2	R	27	GLN
2	R	30	SER
2	R	45	LYS
2	R	47	LEU
2	R	78	LEU
2	R	95	LEU
2	R	125	LEU
2	R	147	GLN
2	R	149	LYS
2	R	201	LEU
2	R	210	ASN

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Mol	Chain	Res	Type
1	S	-1	ILE
1	S	43	LYS
1	S	45	LEU
1	S	73	THR
1	S	138	LEU
1	S	195	ILE
1	S	214	LYS
2	T	24	ARG
2	T	27	GLN
2	T	30	SER
2	T	47	LEU
2	T	72	THR
2	T	125	LEU
2	T	147	GLN
2	T	201	LEU
2	T	210	ASN
1	U	43	LYS
1	U	45	LEU
1	U	73	THR
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
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	210	ASN

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Mol	Chain	Res	Type
1	W	2	VAL
1	W	43	LYS
1	W	45	LEU
1	W	73	THR
1	W	138	LEU
2	X	27	GLN
2	X	30	SER
2	X	47	LEU
2	X	72	THR
2	X	95	LEU
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	m	9	LEU
3	m	10	LEU
3	o	5	LEU
3	o	8	LEU
3	o	9	LEU
3	o	10	LEU
3	q	5	LEU
3	q	15	VAL
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 (124) 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

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Mol	Chain	Res	Type
2	B	27	GLN
2	B	90	GLN
2	B	137	ASN
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	90	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	90	GLN
2	F	100	GLN
2	F	155	GLN
2	F	210	ASN
1	G	28	ASN
1	G	39	GLN
1	G	171	GLN
1	G	197	ASN
1	G	200	HIS
1	H	13	GLN
1	H	28	ASN
1	H	171	GLN
1	H	197	ASN
1	H	200	HIS
2	I	27	GLN
2	I	38	GLN
2	I	90	GLN
2	I	147	GLN
2	I	155	GLN
2	I	160	GLN
2	I	210	ASN
1	J	28	ASN

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Mol	Chain	Res	Type
1	J	171	GLN
1	J	197	ASN
1	J	200	HIS
2	K	27	GLN
2	K	90	GLN
2	K	137	ASN
2	K	155	GLN
2	K	210	ASN
2	L	27	GLN
2	L	90	GLN
2	L	147	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	90	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	90	GLN
2	P	147	GLN
2	P	155	GLN
2	P	160	GLN
1	Q	28	ASN
1	Q	171	GLN
1	Q	197	ASN
1	Q	200	HIS
2	R	27	GLN
2	R	90	GLN
2	R	155	GLN
2	R	160	GLN
2	R	198	HIS
2	R	210	ASN
1	S	28	ASN

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Mol	Chain	Res	Type
1	S	171	GLN
1	S	197	ASN
1	S	200	HIS
2	T	27	GLN
2	T	90	GLN
2	T	155	GLN
2	T	160	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	90	GLN
2	V	100	GLN
2	V	155	GLN
2	V	199	GLN
2	V	210	ASN
1	W	13	GLN
1	W	28	ASN
1	W	171	GLN
1	W	197	ASN
1	W	200	HIS
2	X	27	GLN
2	X	90	GLN
2	X	100	GLN
2	X	155	GLN
2	X	210	ASN
3	a	1	ASN
3	h	1	ASN
3	j	1	ASN
3	j	16	GLN
3	q	1	ASN
3	q	16	GLN
3	q	17	HIS
3	u	1	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	R	301	-	1,3,3	0.37	0	0,3,3	-	-
4	NO3	T	301	-	1,3,3	0.45	0	0,3,3	-	-
4	NO3	I	301	-	1,3,3	0.35	0	0,3,3	-	-
4	NO3	L	301	-	1,3,3	0.26	0	0,3,3	-	-
5	EDO	N	301	-	3,3,3	0.51	0	2,2,2	0.13	0
4	NO3	N	302	-	1,3,3	0.44	0	0,3,3	-	-
4	NO3	D	301	-	1,3,3	0.30	0	0,3,3	-	-
4	NO3	V	301	-	1,3,3	0.33	0	0,3,3	-	-
4	NO3	K	301	-	1,3,3	0.46	0	0,3,3	-	-
4	NO3	B	301	-	1,3,3	0.32	0	0,3,3	-	-
4	NO3	F	301	-	1,3,3	0.37	0	0,3,3	-	-
4	NO3	P	301	-	1,3,3	0.29	0	0,3,3	-	-
4	NO3	X	301	-	1,3,3	0.35	0	0,3,3	-	-
5	EDO	Q	301	-	3,3,3	0.42	0	2,2,2	0.21	0
5	EDO	W	301	-	3,3,3	0.28	0	2,2,2	0.50	0

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	Q	301	-	-	0/1/1/1	-
5	EDO	W	301	-	-	1/1/1/1	-
5	EDO	N	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	W	301	EDO	O1-C1-C2-O2
5	N	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, 95th 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%)	0.17	7 (3%) 50 46	30, 45, 74, 109	0
1	C	219/229 (95%)	0.09	5 (2%) 61 57	24, 36, 67, 108	0
1	E	212/229 (92%)	1.16	47 (22%) 2 2	38, 61, 111, 133	0
1	G	218/229 (95%)	0.12	8 (3%) 45 40	29, 39, 59, 122	0
1	H	219/229 (95%)	-0.00	2 (0%) 81 78	25, 36, 62, 81	0
1	J	224/229 (97%)	0.44	21 (9%) 14 12	27, 46, 90, 110	0
1	M	220/229 (96%)	-0.01	4 (1%) 67 64	24, 36, 59, 109	0
1	O	223/229 (97%)	0.45	12 (5%) 31 27	36, 47, 76, 108	0
1	Q	217/229 (94%)	0.13	4 (1%) 67 64	24, 40, 75, 101	0
1	S	215/229 (93%)	0.62	23 (10%) 11 9	30, 49, 91, 113	0
1	U	217/229 (94%)	1.06	48 (22%) 2 2	34, 52, 125, 144	0
1	W	218/229 (95%)	0.19	7 (3%) 50 46	31, 44, 63, 118	0
2	B	210/215 (97%)	0.50	9 (4%) 40 35	42, 56, 73, 101	0
2	D	210/215 (97%)	0.28	4 (1%) 66 62	30, 42, 61, 101	0
2	F	207/215 (96%)	1.42	52 (25%) 1 1	45, 71, 97, 107	0
2	I	211/215 (98%)	0.18	5 (2%) 59 55	31, 42, 63, 104	0
2	K	210/215 (97%)	0.39	9 (4%) 40 35	29, 48, 72, 97	0
2	L	209/215 (97%)	0.21	4 (1%) 66 62	31, 43, 61, 93	0
2	N	210/215 (97%)	0.25	5 (2%) 59 55	30, 41, 60, 90	0
2	P	210/215 (97%)	0.45	7 (3%) 49 45	32, 50, 74, 90	0
2	R	211/215 (98%)	0.12	6 (2%) 55 50	25, 39, 61, 107	0
2	T	210/215 (97%)	1.01	32 (15%) 5 4	38, 59, 82, 111	0
2	V	210/215 (97%)	1.74	72 (34%) 1 1	50, 68, 99, 114	0
2	X	210/215 (97%)	0.36	6 (2%) 53 49	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%)	1.67	4 (33%) 1 1	64, 75, 88, 94	0
3	c	16/19 (84%)	1.68	3 (18%) 3 2	57, 75, 101, 107	0
3	e	13/19 (68%)	1.12	3 (23%) 2 1	57, 68, 85, 90	0
3	g	13/19 (68%)	1.23	2 (15%) 5 4	60, 71, 88, 93	0
3	h	12/19 (63%)	2.15	5 (41%) 0 0	77, 87, 97, 99	0
3	j	19/19 (100%)	1.05	4 (21%) 2 2	43, 55, 83, 89	0
3	m	13/19 (68%)	0.97	2 (15%) 5 4	51, 59, 72, 80	0
3	o	12/19 (63%)	2.35	8 (66%) 0 0	88, 96, 107, 113	0
3	q	19/19 (100%)	0.93	1 (5%) 32 28	42, 53, 79, 80	0
3	s	12/19 (63%)	0.99	2 (16%) 4 3	51, 65, 86, 86	0
3	u	13/19 (68%)	1.89	6 (46%) 0 0	76, 84, 99, 124	0
3	w	12/19 (63%)	1.81	4 (33%) 1 1	72, 83, 95, 105	0
All	All	5303/5556 (95%)	0.50	443 (8%) 17 15	24, 46, 88, 144	0

All (443) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	137	ALA	7.4
2	V	110	VAL	6.6
1	U	136	ALA	6.2
3	h	12	LEU	5.6
1	S	-1	ILE	5.6
2	F	191	VAL	5.3
1	U	133	GLY	5.1
2	B	29	VAL	5.1
2	V	141	PRO	5.0
2	T	193	ALA	4.9
1	G	133	GLY	4.9
1	U	135	THR	4.8
1	U	161	SER	4.8
3	o	12	LEU	4.8
2	F	192	TYR	4.8
1	U	183	THR	4.8
1	O	133	GLY	4.6
1	U	194	TYR	4.6
2	N	29	VAL	4.5
1	U	154	TRP	4.5
1	U	184	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	V	14	SER	4.4
2	V	111	ALA	4.4
1	U	162	GLY	4.3
1	J	-1	ILE	4.3
1	E	194	TYR	4.2
2	R	4	MET	4.2
2	V	15	VAL	4.2
2	X	5	THR	4.1
2	F	116	PHE	4.1
2	F	211	ARG	4.0
2	V	204	PRO	4.0
1	U	138	LEU	4.0
1	E	136	ALA	4.0
3	w	12	LEU	4.0
2	P	214	CYS	3.9
1	E	195	ILE	3.9
2	N	5	THR	3.9
2	V	78	LEU	3.9
1	U	160	THR	3.9
2	V	200	GLY	3.8
1	U	186	SER	3.8
1	J	191	THR	3.8
2	V	140	TYR	3.8
1	E	189	LEU	3.8
2	P	29	VAL	3.7
2	V	139	PHE	3.7
2	L	5	THR	3.7
1	U	134	GLY	3.7
2	F	154	LEU	3.7
2	V	202	SER	3.7
3	o	1	ASN	3.7
2	V	114	SER	3.7
2	L	29	VAL	3.6
2	V	112	ALA	3.6
2	V	135	LEU	3.6
1	U	182	VAL	3.6
2	F	190	LYS	3.6
2	V	205	VAL	3.5
1	H	133	GLY	3.5
2	F	153	ALA	3.5
1	U	211	VAL	3.5
2	T	205	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	Q	134	GLY	3.5
2	F	119	PRO	3.5
2	R	5	THR	3.5
2	V	116	PHE	3.5
1	E	134	GLY	3.4
2	V	197	THR	3.4
1	U	159	LEU	3.4
1	U	127	SER	3.4
2	V	143	GLU	3.4
1	U	181	VAL	3.4
2	I	212	GLY	3.4
1	E	138	LEU	3.4
1	G	213	PRO	3.4
2	T	202	SER	3.4
2	T	192	TYR	3.3
2	V	173	TYR	3.3
2	B	5	THR	3.3
2	F	29	VAL	3.3
2	V	115	VAL	3.3
3	h	10	LEU	3.3
2	P	5	THR	3.3
1	E	125	ALA	3.3
1	E	209	LYS	3.3
1	U	213	PRO	3.3
1	S	195	ILE	3.3
1	U	195	ILE	3.3
1	W	127	SER	3.3
1	E	135	THR	3.3
2	F	197	THR	3.3
1	E	121	VAL	3.3
2	F	148	TRP	3.3
2	T	111	ALA	3.3
1	E	124	LEU	3.2
1	S	213	PRO	3.2
2	V	5	THR	3.2
2	T	152	ASN	3.2
1	G	216	CYS	3.2
1	E	158	ALA	3.2
1	E	127	SER	3.2
1	J	190	GLY	3.2
2	K	212	GLY	3.2
2	V	146	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	208	SER	3.2
1	E	213	PRO	3.2
3	a	8	LEU	3.2
2	V	106	ILE	3.2
1	E	123	PRO	3.1
3	u	12	LEU	3.1
1	W	216	CYS	3.1
1	E	126	PRO	3.1
1	J	185	PRO	3.1
1	E	211	VAL	3.1
2	F	133	VAL	3.1
2	F	150	VAL	3.1
1	J	217	ASP	3.1
2	V	137	ASN	3.1
1	U	152	VAL	3.1
2	V	144	ALA	3.1
2	F	209	PHE	3.1
2	T	29	VAL	3.1
1	U	193	THR	3.0
1	U	126	PRO	3.0
2	V	154	LEU	3.0
2	F	117	ILE	3.0
1	J	131	THR	3.0
2	I	5	THR	3.0
2	V	198	HIS	3.0
1	U	155	ASN	3.0
1	S	211	VAL	3.0
2	X	29	VAL	3.0
1	E	191	THR	3.0
2	D	5	THR	3.0
1	U	125	ALA	3.0
1	E	185	PRO	3.0
2	V	83	PHE	3.0
1	O	134	GLY	3.0
1	E	137	ALA	3.0
2	F	189	HIS	3.0
1	E	214	LYS	3.0
1	C	161	SER	3.0
1	W	128	SER	3.0
2	I	214	CYS	3.0
2	K	191	VAL	2.9
2	V	142	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	T	209	PHE	2.9
2	V	147	GLN	2.9
1	U	163	VAL	2.9
2	F	193	ALA	2.9
1	A	128	SER	2.9
1	S	190	GLY	2.9
1	U	0	SER	2.9
2	R	30	SER	2.9
3	u	13	ASN	2.9
1	S	137	ALA	2.9
2	V	136	LEU	2.9
1	G	134	GLY	2.9
1	U	157	GLY	2.9
1	E	198	VAL	2.9
2	V	13	ALA	2.9
2	N	68	GLY	2.9
1	E	182	VAL	2.8
2	F	132	VAL	2.8
2	V	214	CYS	2.8
1	U	199	ASN	2.8
1	U	123	PRO	2.8
1	S	193	THR	2.8
2	F	5	THR	2.8
3	s	12	LEU	2.8
1	S	122	PHE	2.8
2	V	171	SER	2.8
2	F	206	THR	2.8
2	V	69	THR	2.8
3	o	8	LEU	2.8
1	M	128	SER	2.8
2	T	110	VAL	2.8
1	U	158	ALA	2.8
2	F	127	SER	2.7
1	U	198	VAL	2.7
2	F	205	VAL	2.7
2	K	5	THR	2.7
2	V	172	THR	2.7
1	S	209	LYS	2.7
2	T	190	LYS	2.7
2	K	214	CYS	2.7
1	S	127	SER	2.7
2	V	203	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	U	189	LEU	2.7
2	T	5	THR	2.7
1	E	122	PHE	2.7
1	W	126	PRO	2.7
2	V	138	ASN	2.7
1	C	130	SER	2.7
2	D	29	VAL	2.7
2	F	202	SER	2.7
2	I	29	VAL	2.7
2	R	77	SER	2.7
2	V	175	LEU	2.7
3	a	10	LEU	2.7
2	F	118	PHE	2.7
1	G	204	ASN	2.7
1	G	128	SER	2.7
2	R	29	VAL	2.7
2	T	31	SER	2.7
2	V	12	SER	2.7
2	T	200	GLY	2.6
1	A	216	CYS	2.6
1	J	213	PRO	2.6
1	U	214	LYS	2.6
2	V	145	LYS	2.6
3	j	19	PRO	2.6
2	F	210	ASN	2.6
2	L	152	ASN	2.6
2	V	11	LEU	2.6
1	E	161	SER	2.6
1	E	188	SER	2.6
3	c	15	VAL	2.6
1	S	138	LEU	2.6
1	U	196	CYS	2.6
2	D	214	CYS	2.6
3	a	1	ASN	2.6
1	O	0	SER	2.6
1	U	156	SER	2.6
1	W	0	SER	2.6
1	S	136	ALA	2.6
2	I	152	ASN	2.6
2	N	27	GLN	2.6
2	X	214	CYS	2.6
3	c	16	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	T	112	ALA	2.6
2	V	107	LYS	2.6
1	O	217	ASP	2.5
3	o	10	LEU	2.5
2	V	163	VAL	2.5
1	O	130	SER	2.5
2	B	69	THR	2.5
1	S	181	VAL	2.5
1	S	214	LYS	2.5
3	j	17	HIS	2.5
2	T	171	SER	2.5
2	T	214	CYS	2.5
2	V	80	PRO	2.5
2	V	82	ASP	2.5
2	T	125	LEU	2.5
2	V	62	PHE	2.5
2	T	153	ALA	2.5
1	E	179	SER	2.5
2	T	206	THR	2.5
2	R	214	CYS	2.5
3	o	11	GLU	2.5
2	V	17	ASP	2.5
2	F	201	LEU	2.5
2	F	207	LYS	2.5
1	U	166	PHE	2.5
2	F	196	VAL	2.5
1	M	0	SER	2.5
2	V	22	THR	2.5
1	E	190	GLY	2.4
1	J	214	LYS	2.4
2	F	181	LEU	2.4
3	o	5	LEU	2.4
2	V	108	ARG	2.4
2	F	115	VAL	2.4
3	q	14	ALA	2.4
2	V	20	THR	2.4
2	V	109	THR	2.4
1	O	215	SER	2.4
1	S	215	SER	2.4
2	F	134	CYS	2.4
3	c	12	LEU	2.4
3	h	5	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	u	8	LEU	2.4
1	J	29	VAL	2.4
2	V	19	VAL	2.4
2	V	29	VAL	2.4
1	J	187	SER	2.4
1	O	132	SER	2.4
1	O	214	LYS	2.4
2	F	188	LYS	2.4
1	O	216	CYS	2.4
1	U	197	ASN	2.4
1	J	209	LYS	2.4
2	B	190	LYS	2.4
1	A	0	SER	2.4
2	F	136	LEU	2.4
2	F	186	TYR	2.4
1	E	155	ASN	2.4
3	g	1	ASN	2.4
3	j	18	ASN	2.4
2	F	114	SER	2.3
2	P	28	SER	2.3
2	V	162	SER	2.3
2	X	30	SER	2.3
1	E	162	GLY	2.3
2	F	179	LEU	2.3
1	A	92	CYS	2.3
2	F	194	CYS	2.3
2	V	134	CYS	2.3
1	J	184	VAL	2.3
1	U	207	VAL	2.3
2	V	206	THR	2.3
1	E	0	SER	2.3
1	O	187	SER	2.3
2	B	76	SER	2.3
2	P	30	SER	2.3
1	S	162	GLY	2.3
2	B	212	GLY	2.3
2	F	157	GLY	2.3
2	F	155	GLN	2.3
2	P	106	ILE	2.3
3	e	8	LEU	2.3
3	h	9	LEU	2.3
3	o	9	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	204	ASN	2.3
1	A	158	ALA	2.3
2	V	74	THR	2.3
1	E	174	GLY	2.3
2	N	31	SER	2.3
2	X	213	GLU	2.3
2	V	49	TYR	2.3
1	J	128	SER	2.3
1	U	164	HIS	2.3
2	V	16	GLY	2.3
2	F	76	SER	2.3
2	L	31	SER	2.3
2	T	208	SER	2.3
2	F	147	GLN	2.2
2	T	189	HIS	2.2
1	J	0	SER	2.2
1	J	132	SER	2.2
1	J	159	LEU	2.2
2	V	207	LYS	2.2
1	C	213	PRO	2.2
2	B	214	CYS	2.2
1	J	73	THR	2.2
1	U	191	THR	2.2
1	M	129	LYS	2.2
2	X	212	GLY	2.2
2	T	201	LEU	2.2
1	J	130	SER	2.2
1	U	187	SER	2.2
1	E	154	TRP	2.2
2	K	213	GLU	2.2
3	w	11	GLU	2.2
3	m	1	ASN	2.2
1	U	216	CYS	2.2
2	V	6	GLN	2.2
3	e	12	LEU	2.2
3	w	10	LEU	2.2
1	E	74	SER	2.2
1	S	179	SER	2.2
1	E	1	GLU	2.2
3	o	4	GLU	2.2
1	E	184	VAL	2.2
3	j	15	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	214	LYS	2.2
1	W	214	LYS	2.2
2	T	144	ALA	2.2
2	V	166	GLN	2.2
2	V	199	GLN	2.2
2	T	134	CYS	2.2
3	g	10	LEU	2.2
1	A	127	SER	2.2
1	G	0	SER	2.2
2	V	77	SER	2.2
3	u	3	SER	2.2
1	O	129	LYS	2.2
2	K	29	VAL	2.1
3	s	1	ASN	2.1
2	F	135	LEU	2.1
2	P	68	GLY	2.1
1	E	186	SER	2.1
2	F	151	ASP	2.1
2	K	122	ASP	2.1
2	T	28	SER	2.1
2	V	63	SER	2.1
1	U	185	PRO	2.1
2	V	118	PHE	2.1
1	E	142	VAL	2.1
1	E	181	VAL	2.1
1	S	184	VAL	2.1
2	V	104	VAL	2.1
1	E	8	GLY	2.1
1	E	175	LEU	2.1
2	F	129	THR	2.1
2	F	175	LEU	2.1
3	a	12	LEU	2.1
1	U	212	GLU	2.1
2	T	140	TYR	2.1
1	J	215	SER	2.1
1	U	203	SER	2.1
2	F	156	SER	2.1
2	F	149	LYS	2.1
1	S	207	VAL	2.1
2	T	115	VAL	2.1
2	T	191	VAL	2.1
2	T	148	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	152	ASN	2.1
3	w	8	LEU	2.1
2	D	187	GLU	2.1
1	O	31	TYR	2.1
1	M	127	SER	2.1
1	W	215	SER	2.1
2	K	30	SER	2.1
1	S	189	LEU	2.1
2	B	18	ARG	2.1
3	u	2	LEU	2.1
1	J	193	THR	2.1
2	F	180	THR	2.1
1	C	129	LYS	2.1
1	C	214	LYS	2.1
1	J	206	LYS	2.1
1	S	208	ASP	2.1
2	F	70	ASP	2.1
2	B	28	SER	2.1
1	E	140	CYS	2.1
1	Q	216	CYS	2.1
2	F	146	VAL	2.0
1	S	141	LEU	2.0
3	e	1	ASN	2.0
3	m	13	ASN	2.0
2	F	195	GLU	2.0
1	U	210	LYS	2.0
1	Q	217	ASP	2.0
1	E	119	PRO	2.0
1	Q	215	SER	2.0
2	T	30	SER	2.0
1	E	196	CYS	2.0
1	E	212	GLU	2.0
1	S	212	GLU	2.0
2	V	47	LEU	2.0
3	h	8	LEU	2.0
2	T	207	LYS	2.0
2	V	68	GLY	2.0
3	u	1	ASN	2.0
1	H	131	THR	2.0
2	T	109	THR	2.0
2	V	113	PRO	2.0
1	A	215	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	156	SER	2.0
2	V	9	SER	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 oligosaccharides 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, 95th 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
4	NO3	V	301	4/4	0.73	0.21	37,39,39,39	4
4	NO3	B	301	4/4	0.84	0.19	59,59,63,66	0
4	NO3	P	301	4/4	0.86	0.13	30,31,31,32	4
5	EDO	W	301	4/4	0.86	0.15	47,47,48,48	0
4	NO3	L	301	4/4	0.87	0.17	26,26,27,27	4
5	EDO	N	301	4/4	0.89	0.12	38,39,39,40	0
4	NO3	F	301	4/4	0.89	0.14	26,26,27,28	4
4	NO3	I	301	4/4	0.90	0.14	49,49,52,55	0
4	NO3	K	301	4/4	0.91	0.17	41,42,42,47	0
4	NO3	X	301	4/4	0.93	0.12	47,49,49,50	0
4	NO3	D	301	4/4	0.95	0.16	41,45,45,47	0
4	NO3	T	301	4/4	0.95	0.11	22,23,23,23	4
5	EDO	Q	301	4/4	0.95	0.09	32,33,33,33	0
4	NO3	N	302	4/4	0.95	0.07	41,42,43,45	0
4	NO3	R	301	4/4	0.97	0.10	38,38,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.