



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:19 PM UTC

PDB ID : 4ZYP / pdb_00004zyp
Title : Crystal Structure of Motavizumab and Quaternary-Specific RSV-Neutralizing Human Antibody AM14 in Complex with Prefusion RSV F Glycoprotein
Authors : Gilman, M.S.A.; McLellan, J.S.
Deposited on : 2015-05-21
Resolution : 5.50 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
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

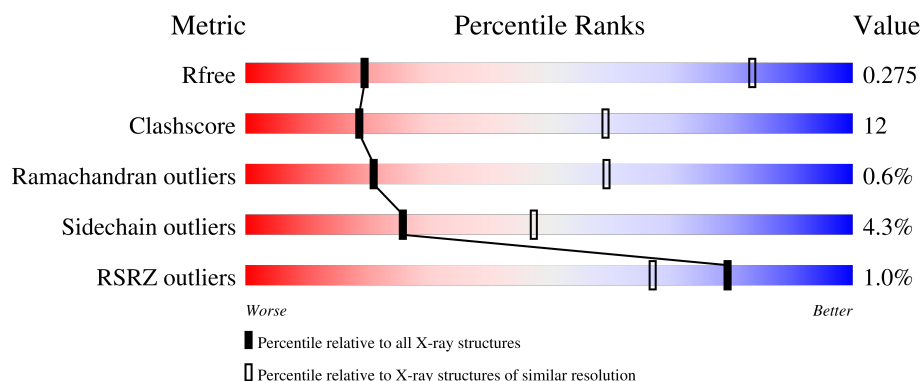
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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.



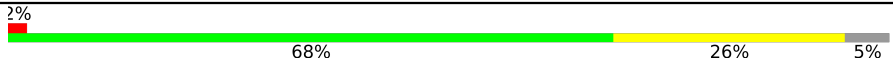
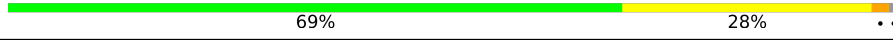
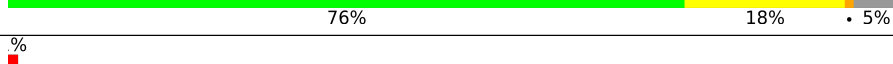
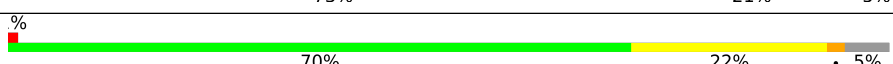
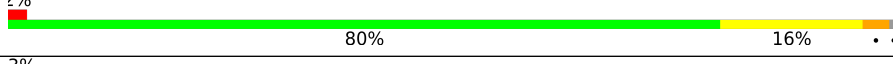
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

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	498	% 56% 31% • 10%
1	B	498	56% 29% 5% 10%
1	C	498	% 55% 30% • 10%
2	J	225	% 56% 34% • 5%
2	K	225	56% 35% • 5%

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Mol	Chain	Length	Quality of chain
2	N	225	
3	L	213	
3	M	213	
3	O	213	
4	D	227	
4	F	227	
4	H	227	
5	E	215	
5	G	215	
5	I	215	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29990 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 Fusion glycoprotein F0,Fibritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3482	2202	573	684	23			
1	B	449	Total	C	N	O	S	0	0	0
			3482	2202	573	684	23			
1	C	449	Total	C	N	O	S	0	0	0
			3482	2202	573	684	23			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ALA	PRO	conflict	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	GLU	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	PRO	deletion	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	PHE	deletion	UNP P03420
A	?	-	MET	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	TYR	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ALA	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	VAL	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	155	CYS	SER	engineered mutation	UNP P03420
A	190	PHE	SER	engineered mutation	UNP P03420
A	207	LEU	VAL	engineered mutation	UNP P03420
A	290	CYS	SER	engineered mutation	UNP P03420
A	379	VAL	ILE	engineered mutation	UNP P03420
A	447	VAL	MET	engineered mutation	UNP P03420
A	514	SER	-	linker	UNP P03420
A	515	ALA	-	linker	UNP P03420
A	516	ILE	-	linker	UNP P03420
A	517	GLY	-	linker	UNP P03420
A	545	GLY	-	expression tag	UNP D9IEJ2
A	546	GLY	-	expression tag	UNP D9IEJ2
A	547	LEU	-	expression tag	UNP D9IEJ2
A	548	VAL	-	expression tag	UNP D9IEJ2
A	549	PRO	-	expression tag	UNP D9IEJ2
A	550	ARG	-	expression tag	UNP D9IEJ2
B	129	ALA	PRO	conflict	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	GLU	deletion	UNP P03420
B	?	-	LEU	deletion	UNP P03420
B	?	-	PRO	deletion	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	PHE	deletion	UNP P03420
B	?	-	MET	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	TYR	deletion	UNP P03420
B	?	-	THR	deletion	UNP P03420
B	?	-	LEU	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	ALA	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	THR	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	VAL	deletion	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P03420
B	?	-	LEU	deletion	UNP P03420
B	?	-	SER	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	155	CYS	SER	engineered mutation	UNP P03420
B	190	PHE	SER	engineered mutation	UNP P03420
B	207	LEU	VAL	engineered mutation	UNP P03420
B	290	CYS	SER	engineered mutation	UNP P03420
B	379	VAL	ILE	engineered mutation	UNP P03420
B	447	VAL	MET	engineered mutation	UNP P03420
B	514	SER	-	linker	UNP P03420
B	515	ALA	-	linker	UNP P03420
B	516	ILE	-	linker	UNP P03420
B	517	GLY	-	linker	UNP P03420
B	545	GLY	-	expression tag	UNP D9IEJ2
B	546	GLY	-	expression tag	UNP D9IEJ2
B	547	LEU	-	expression tag	UNP D9IEJ2
B	548	VAL	-	expression tag	UNP D9IEJ2
B	549	PRO	-	expression tag	UNP D9IEJ2
B	550	ARG	-	expression tag	UNP D9IEJ2
C	129	ALA	PRO	conflict	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	GLU	deletion	UNP P03420
C	?	-	LEU	deletion	UNP P03420
C	?	-	PRO	deletion	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	PHE	deletion	UNP P03420
C	?	-	MET	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	TYR	deletion	UNP P03420
C	?	-	THR	deletion	UNP P03420
C	?	-	LEU	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	ALA	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	THR	deletion	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASN	deletion	UNP P03420
C	?	-	VAL	deletion	UNP P03420
C	?	-	THR	deletion	UNP P03420
C	?	-	LEU	deletion	UNP P03420
C	?	-	SER	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	155	CYS	SER	engineered mutation	UNP P03420
C	190	PHE	SER	engineered mutation	UNP P03420
C	207	LEU	VAL	engineered mutation	UNP P03420
C	290	CYS	SER	engineered mutation	UNP P03420
C	379	VAL	ILE	engineered mutation	UNP P03420
C	447	VAL	MET	engineered mutation	UNP P03420
C	514	SER	-	linker	UNP P03420
C	515	ALA	-	linker	UNP P03420
C	516	ILE	-	linker	UNP P03420
C	517	GLY	-	linker	UNP P03420
C	545	GLY	-	expression tag	UNP D9IEJ2
C	546	GLY	-	expression tag	UNP D9IEJ2
C	547	LEU	-	expression tag	UNP D9IEJ2
C	548	VAL	-	expression tag	UNP D9IEJ2
C	549	PRO	-	expression tag	UNP D9IEJ2
C	550	ARG	-	expression tag	UNP D9IEJ2

- Molecule 2 is a protein called Motavizumab antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	213	Total	C	N	O	S	0	0	0
			1626	1039	266	314	7			
2	K	213	Total	C	N	O	S	0	0	0
			1626	1039	266	314	7			
2	N	213	Total	C	N	O	S	0	0	0
			1626	1039	266	314	7			

- Molecule 3 is a protein called Motavizumab antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1611	1012	268	325	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	211	Total	C	N	O	S	0	0	0
			1611	1012	268	325	6			
3	O	211	Total	C	N	O	S	0	0	0
			1611	1012	268	325	6			

- Molecule 4 is a protein called AM14 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	216	Total	C	N	O	S	0	0	0
			1636	1033	276	320	7			
4	H	216	Total	C	N	O	S	0	0	0
			1635	1033	276	319	7			
4	D	216	Total	C	N	O	S	0	0	0
			1636	1033	276	320	7			

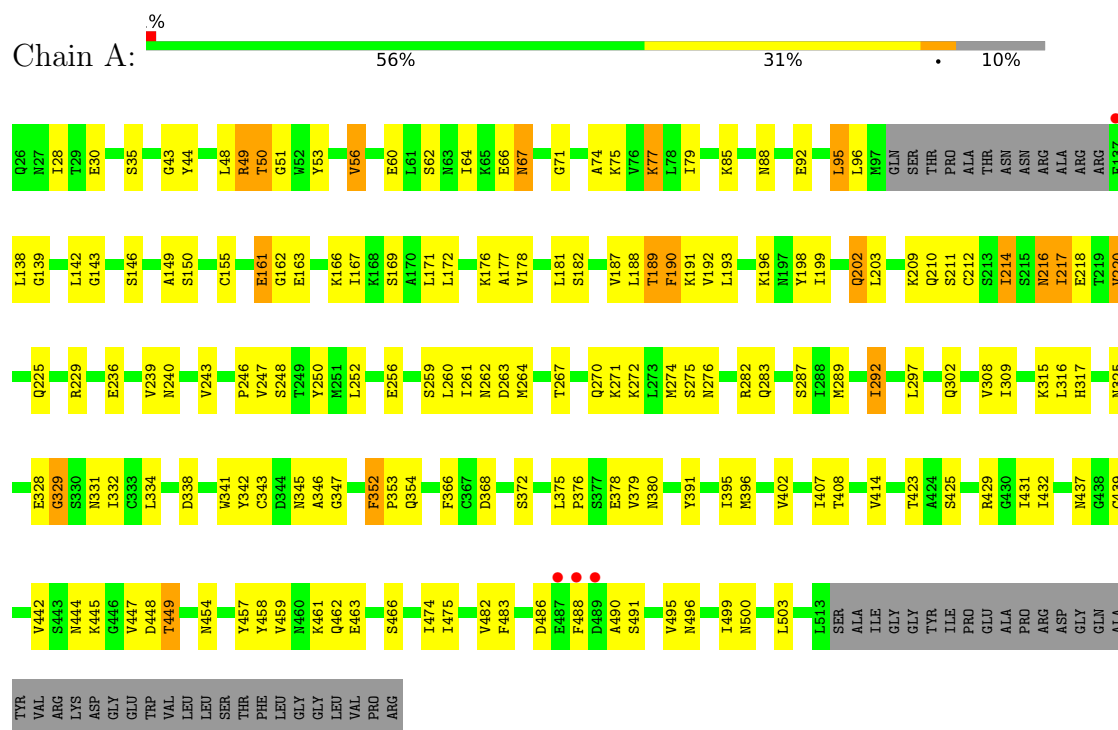
- Molecule 5 is a protein called AM14 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	213	Total	C	N	O	S	0	0	0
			1642	1025	277	334	6			
5	I	213	Total	C	N	O	S	0	0	0
			1642	1025	277	334	6			
5	E	213	Total	C	N	O	S	0	0	0
			1642	1025	277	334	6			

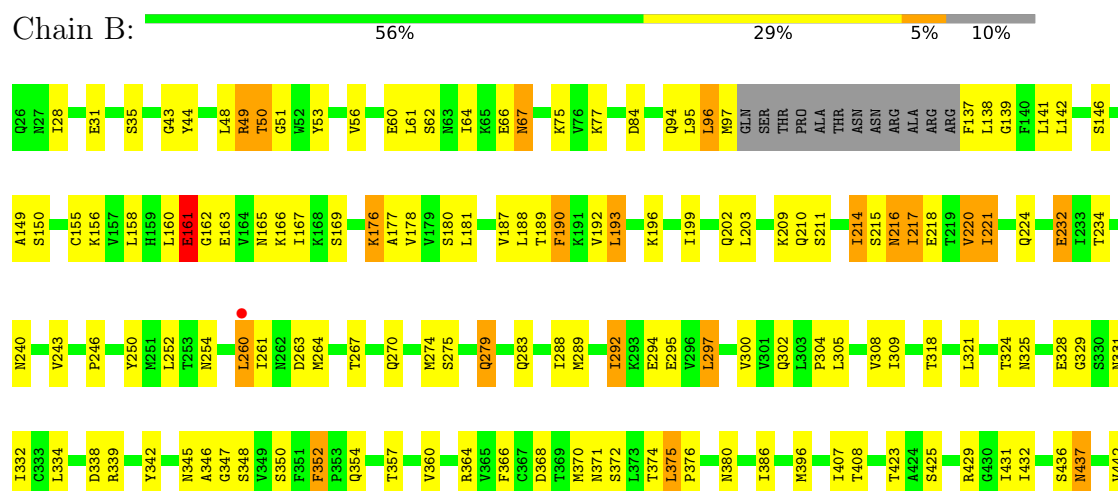
3 Residue-property plots

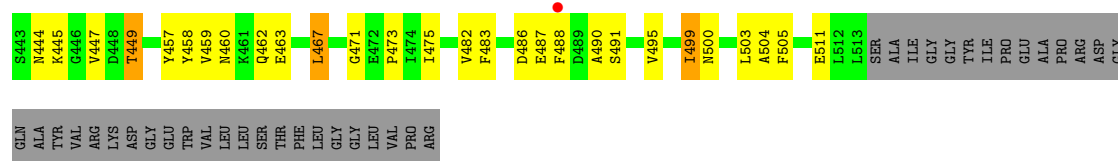
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Fusion glycoprotein F0,Fibritin

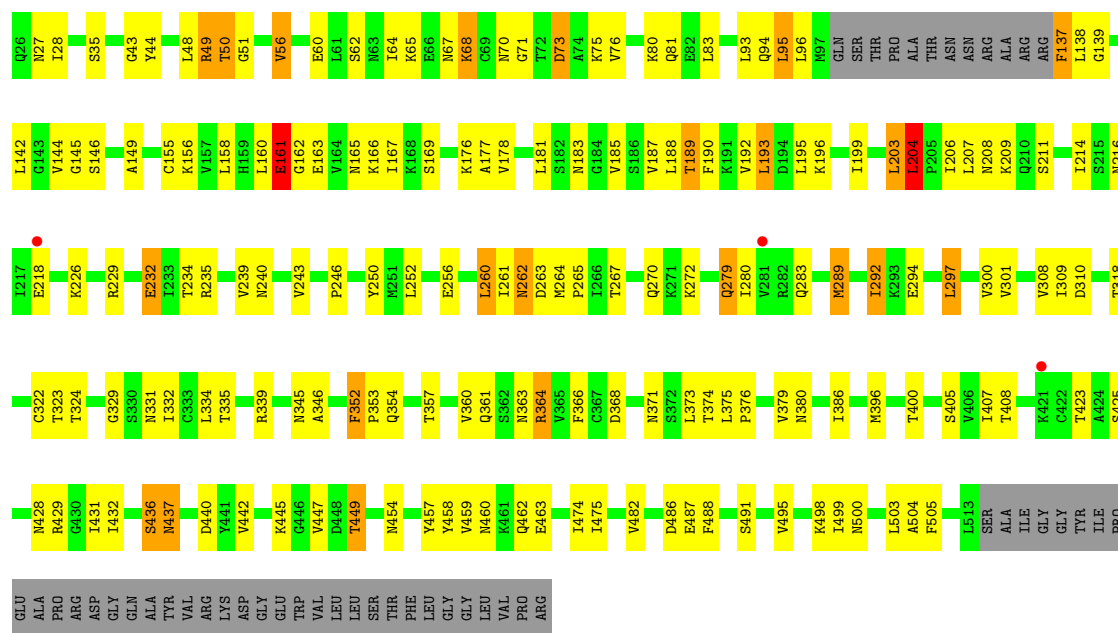


• Molecule 1: Fusion glycoprotein F0,Fibritin

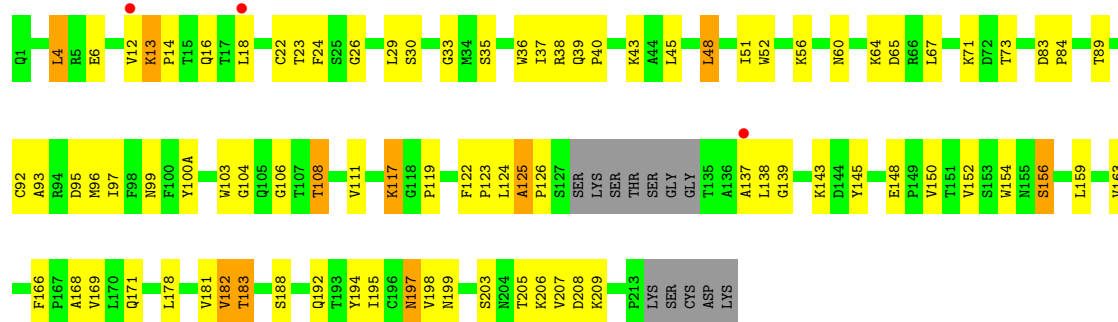




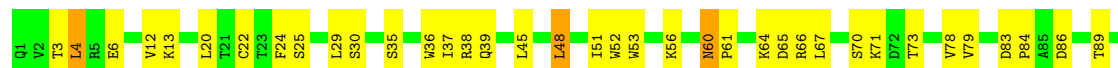
• Molecule 1: Fusion glycoprotein F0, Fibrinogen

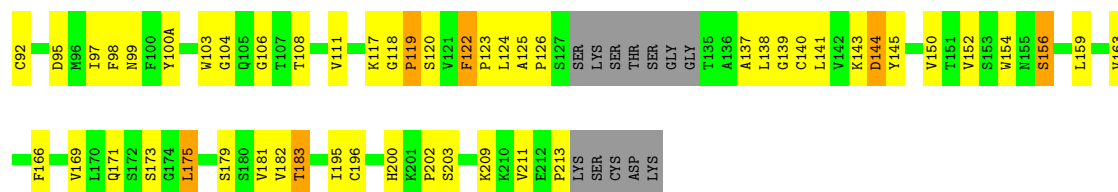


• Molecule 2: Motavizumab antibody Fab heavy chain

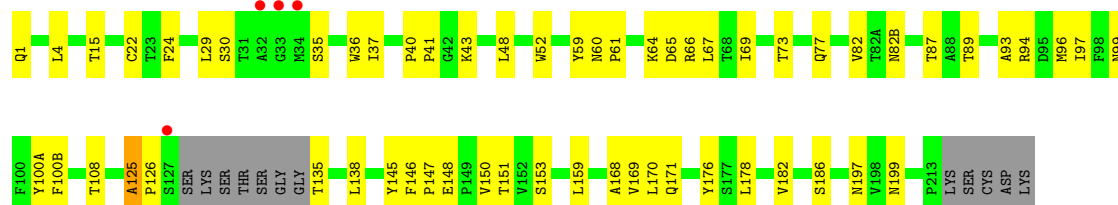


• Molecule 2: Motavizumab antibody Fab heavy chain

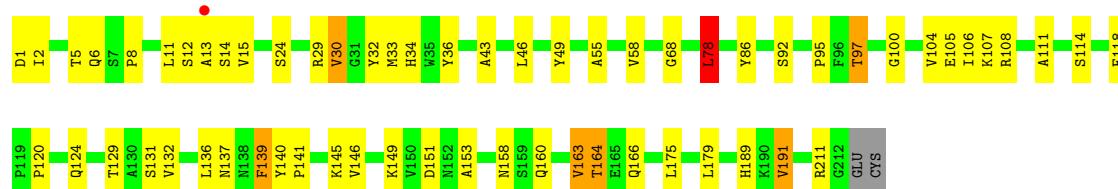




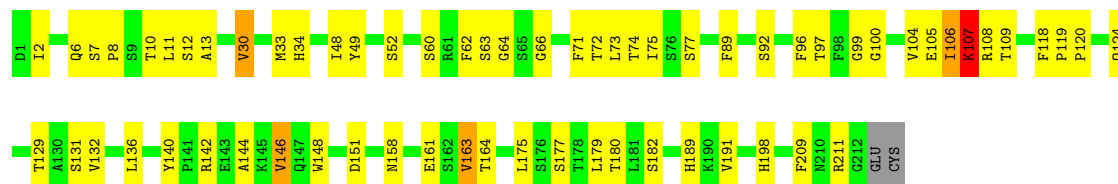
• Molecule 2: Motavizumab antibody Fab heavy chain



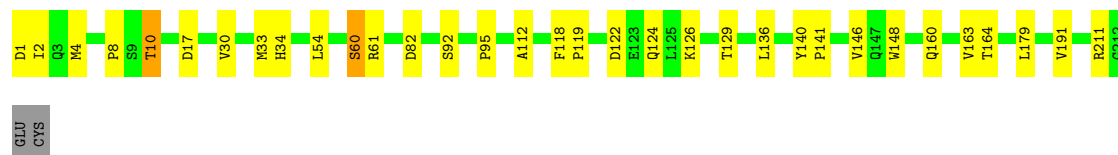
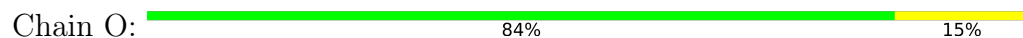
• Molecule 3: Motavizumab antibody light chain



• Molecule 3: Motavizumab antibody light chain

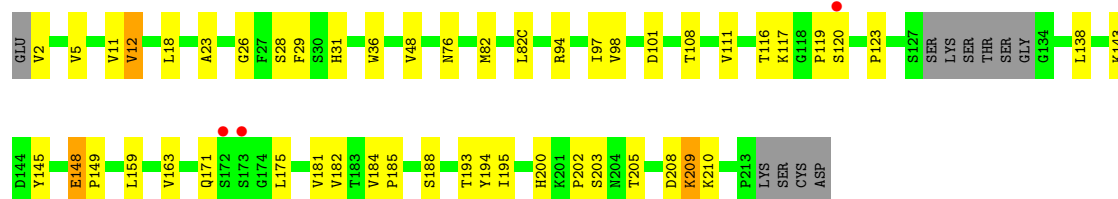


• Molecule 3: Motavizumab antibody light chain



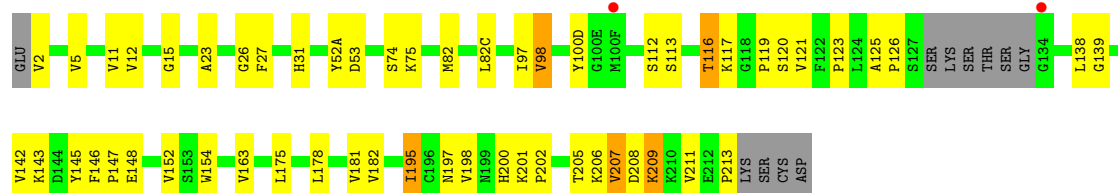
• Molecule 4: AM14 antibody Fab heavy chain

Chain F: 



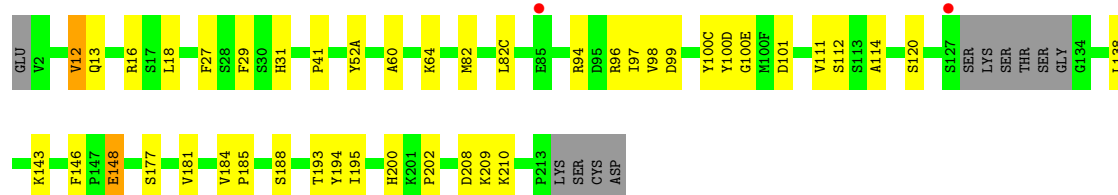
- Molecule 4: AM14 antibody Fab heavy chain

Chain H: 



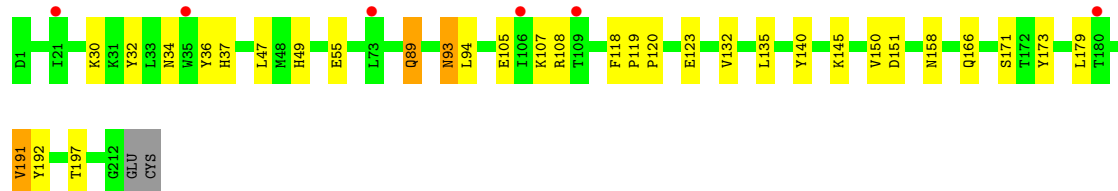
- Molecule 4: AM14 antibody Fab heavy chain

Chain D: 



- Molecule 5: AM14 antibody light chain

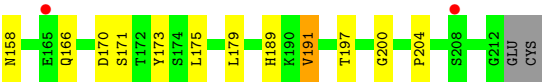
Chain G: 



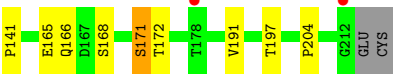
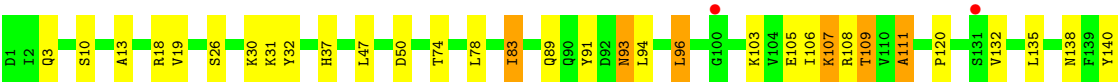
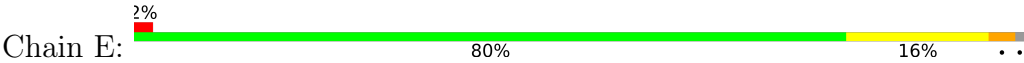
- Molecule 5: AM14 antibody light chain

Chain I: 





● Molecule 5: AM14 antibody light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.38Å 210.29Å 118.20Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	49.39 – 5.50 49.39 – 5.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.39-5.50) 97.1 (49.39-5.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 5.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.277 0.215 , 0.275	Depositor DCC
R_{free} test set	857 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	154.0	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 247.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.056 for l,-k,h	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29990	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

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	0.46	0/3532	1.09	22/4784 (0.5%)
1	B	0.46	0/3532	1.10	24/4784 (0.5%)
1	C	0.48	0/3532	1.13	23/4784 (0.5%)
2	J	0.54	0/1669	1.41	35/2283 (1.5%)
2	K	0.43	0/1669	1.26	29/2283 (1.3%)
2	N	0.38	0/1669	0.84	4/2283 (0.2%)
3	L	0.47	0/1648	1.11	9/2235 (0.4%)
3	M	0.46	0/1648	1.16	7/2235 (0.3%)
3	O	0.39	0/1648	0.86	3/2235 (0.1%)
4	D	0.36	0/1677	0.83	1/2286 (0.0%)
4	F	0.36	0/1677	0.83	0/2286
4	H	0.41	0/1676	1.09	13/2285 (0.6%)
5	E	0.44	0/1677	0.97	8/2277 (0.4%)
5	G	0.35	0/1677	0.80	1/2277 (0.0%)
5	I	0.40	0/1677	0.87	2/2277 (0.1%)
All	All	0.44	0/30608	1.05	181/41594 (0.4%)

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
3	L	0	1

There are no bond length outliers.

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	107	LYS	N-CA-C	11.73	127.61	108.96
2	J	122	PHE	CA-C-N	-10.91	108.20	119.99
2	J	122	PHE	C-N-CA	-10.91	108.20	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	207	VAL	N-CA-C	10.06	122.25	108.17
2	K	169	VAL	N-CA-C	9.85	121.96	108.17
1	B	482	VAL	N-CA-C	-9.85	102.69	113.43
2	J	106	GLY	N-CA-C	9.45	124.59	112.68
3	L	164	THR	N-CA-C	9.39	125.04	110.20
3	M	100	GLY	N-CA-C	-9.20	103.25	114.66
4	H	205	THR	N-CA-C	9.00	122.89	108.41
2	J	166	PHE	CA-C-N	8.94	131.01	119.84
2	J	166	PHE	C-N-CA	8.94	131.01	119.84
1	B	375	LEU	CA-C-N	8.81	128.86	119.78
1	B	375	LEU	C-N-CA	8.81	128.86	119.78
3	L	100	GLY	N-CA-C	-8.71	103.86	114.66
1	C	142	LEU	N-CA-C	8.65	121.66	111.71
1	A	142	LEU	N-CA-C	8.54	121.53	111.71
2	J	13	LYS	CA-C-N	8.25	128.76	119.93
2	J	13	LYS	C-N-CA	8.25	128.76	119.93
2	K	181	VAL	N-CA-C	8.19	119.16	108.35
2	J	181	VAL	N-CA-C	8.18	119.14	108.35
2	J	104	GLY	N-CA-C	-8.13	102.13	112.54
1	C	352	PHE	CA-C-N	8.05	127.34	118.97
1	C	352	PHE	C-N-CA	8.05	127.34	118.97
2	K	104	GLY	N-CA-C	-7.98	103.55	112.33
1	B	347	GLY	N-CA-C	-7.96	104.86	115.21
1	A	483	PHE	CA-C-N	7.86	129.67	119.84
1	A	483	PHE	C-N-CA	7.86	129.67	119.84
1	A	352	PHE	CA-C-N	7.74	127.02	118.97
1	A	352	PHE	C-N-CA	7.74	127.02	118.97
2	J	169	VAL	N-CA-C	7.70	119.37	108.36
1	B	352	PHE	CA-C-N	7.69	126.97	118.97
1	B	352	PHE	C-N-CA	7.69	126.97	118.97
2	J	166	PHE	N-CA-C	7.63	119.85	109.24
1	C	436	SER	N-CA-C	7.59	121.23	110.68
1	A	482	VAL	N-CA-C	-7.54	105.21	113.43
2	N	125	ALA	CA-C-N	7.51	127.44	119.85
2	N	125	ALA	C-N-CA	7.51	127.44	119.85
1	C	482	VAL	N-CA-C	-7.47	105.29	113.43
3	L	58	VAL	CA-C-N	7.44	127.42	119.76
3	L	58	VAL	C-N-CA	7.44	127.42	119.76
2	J	205	THR	N-CA-C	7.44	121.03	108.02
2	J	183	THR	N-CA-C	-7.42	98.91	110.42
2	K	166	PHE	CA-C-N	7.38	129.06	119.84
2	K	166	PHE	C-N-CA	7.38	129.06	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	107	LYS	N-CA-C	7.36	120.67	108.96
2	K	125	ALA	CA-C-N	7.28	127.45	120.31
2	K	125	ALA	C-N-CA	7.28	127.45	120.31
1	C	192	VAL	N-CA-C	7.12	122.75	113.07
1	C	262	ASN	N-CA-C	7.08	119.85	111.71
4	H	125	ALA	CA-C-N	7.08	127.64	120.14
4	H	125	ALA	C-N-CA	7.08	127.64	120.14
2	K	106	GLY	N-CA-C	7.00	121.50	112.68
2	K	122	PHE	CA-C-N	-6.97	112.46	119.99
2	K	122	PHE	C-N-CA	-6.97	112.46	119.99
1	C	375	LEU	CA-C-N	6.97	126.96	119.78
1	C	375	LEU	C-N-CA	6.97	126.96	119.78
1	A	190	PHE	N-CA-C	6.86	119.60	108.34
1	A	328	GLU	N-CA-C	6.75	118.52	111.03
2	J	60	ASN	CA-C-N	6.74	127.29	119.47
2	J	60	ASN	C-N-CA	6.74	127.29	119.47
1	C	211	SER	N-CA-C	6.70	119.61	108.96
2	K	166	PHE	N-CA-C	6.68	118.53	109.24
1	A	375	LEU	CA-C-N	6.67	126.65	119.78
1	A	375	LEU	C-N-CA	6.67	126.65	119.78
2	K	60	ASN	CA-C-N	6.67	127.20	119.47
2	K	60	ASN	C-N-CA	6.67	127.20	119.47
2	J	148	GLU	N-CA-C	-6.58	101.83	110.39
2	J	152	VAL	N-CA-C	6.55	118.22	108.46
2	K	92	CYS	N-CA-C	-6.55	99.24	109.72
5	E	171	SER	N-CA-C	6.41	120.45	112.24
5	E	93	ASN	CB-CA-C	-6.39	108.53	117.23
2	J	92	CYS	N-CA-C	-6.38	99.51	109.72
1	A	44	TYR	N-CA-C	6.33	119.89	110.52
1	C	49	ARG	N-CA-C	6.33	120.72	113.19
1	A	192	VAL	N-CA-C	6.29	121.63	113.07
2	J	207	VAL	N-CA-C	6.28	117.83	108.23
5	I	93	ASN	CB-CA-C	-6.27	108.70	117.23
1	B	436	SER	N-CA-C	6.18	119.28	110.68
1	B	499	ILE	N-CA-C	-6.18	104.48	110.72
1	B	192	VAL	N-CA-C	6.14	120.66	112.98
2	K	103	TRP	CA-C-N	6.14	127.13	120.44
2	K	103	TRP	C-N-CA	6.14	127.13	120.44
2	N	60	ASN	CA-C-N	6.12	126.57	119.47
2	N	60	ASN	C-N-CA	6.12	126.57	119.47
3	O	112	ALA	CA-C-N	6.11	125.87	119.76
3	O	112	ALA	C-N-CA	6.11	125.87	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	183	THR	N-CA-C	-6.11	100.96	110.42
2	J	198	VAL	N-CA-C	6.09	117.35	108.58
1	B	49	ARG	N-CA-C	6.05	120.39	113.19
1	A	347	GLY	N-CA-C	-6.03	107.37	115.21
4	H	98	VAL	N-CA-C	5.98	117.63	108.71
1	A	49	ARG	N-CA-C	5.98	120.31	113.19
5	G	93	ASN	CB-CA-C	-5.98	109.10	117.23
2	K	152	VAL	N-CA-C	5.95	117.33	108.46
2	K	173	SER	N-CA-C	-5.92	106.03	113.20
1	B	360	VAL	N-CA-C	5.91	116.44	108.17
5	E	109	THR	N-CA-C	-5.88	98.27	110.80
4	H	113	SER	N-CA-C	-5.87	104.88	111.28
1	B	142	LEU	N-CA-C	5.86	118.44	111.71
1	A	329	GLY	N-CA-C	-5.84	99.34	113.18
2	J	182	VAL	N-CA-C	5.83	116.33	108.17
2	J	117	LYS	CA-C-N	5.78	130.94	121.87
2	J	117	LYS	C-N-CA	5.78	130.94	121.87
1	C	190	PHE	N-CA-C	5.77	117.80	108.34
3	M	182	SER	N-CA-C	-5.76	102.92	110.53
2	K	150	VAL	CA-C-N	-5.75	113.16	122.36
2	K	150	VAL	C-N-CA	-5.75	113.16	122.36
1	B	44	TYR	N-CA-C	5.74	119.01	110.52
2	J	26	GLY	N-CA-C	-5.68	107.94	114.69
2	K	175	LEU	N-CA-C	5.62	118.84	110.52
1	B	328	GLU	N-CA-C	5.62	117.26	111.03
1	B	84	ASP	N-CA-C	-5.61	104.79	111.69
1	C	366	PHE	N-CA-C	5.61	117.44	108.41
1	C	199	ILE	N-CA-C	5.60	116.38	110.72
1	A	56	VAL	N-CA-C	5.60	115.66	107.37
1	C	360	VAL	N-CA-C	5.60	116.00	108.17
2	J	103	TRP	N-CA-C	5.58	118.19	108.76
1	B	483	PHE	CA-C-N	5.58	126.81	119.84
1	B	483	PHE	C-N-CA	5.58	126.81	119.84
5	E	165	GLU	N-CA-C	-5.57	103.18	110.53
3	M	72	THR	N-CA-C	5.55	118.50	109.06
2	K	13	LYS	CA-C-N	5.55	125.86	119.93
2	K	13	LYS	C-N-CA	5.55	125.86	119.93
1	B	511	GLU	N-CA-C	-5.51	105.35	111.36
1	C	204	LEU	N-CA-C	5.49	121.08	113.45
4	D	112	SER	N-CA-C	5.49	117.43	108.76
3	L	43	ALA	CA-C-N	5.48	125.41	119.76
3	L	43	ALA	C-N-CA	5.48	125.41	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	PHE	N-CA-C	5.47	117.22	108.41
2	J	125	ALA	CA-C-N	5.47	125.67	120.31
2	J	125	ALA	C-N-CA	5.47	125.67	120.31
4	H	125	ALA	N-CA-C	5.42	116.71	109.83
3	O	2	ILE	N-CA-C	5.39	115.62	107.80
1	C	50	THR	N-CA-C	5.37	122.24	110.80
1	B	176	LYS	N-CA-C	5.37	117.17	108.26
1	B	190	PHE	N-CA-C	5.36	117.14	108.34
1	A	343	CYS	N-CA-C	5.36	118.17	109.06
5	I	101	GLY	N-CA-C	5.35	119.35	112.18
2	K	117	LYS	N-CA-C	5.35	116.54	108.46
1	B	50	THR	N-CA-C	5.34	122.19	110.80
5	E	111	ALA	N-CA-C	5.31	117.06	108.34
4	H	206	LYS	CA-C-N	5.30	129.76	123.19
4	H	206	LYS	C-N-CA	5.30	129.76	123.19
4	H	15	GLY	N-CA-C	-5.28	108.41	114.69
1	C	44	TYR	N-CA-C	5.26	118.30	110.52
1	A	50	THR	N-CA-C	5.25	121.99	110.80
1	B	221	ILE	N-CA-C	-5.25	105.60	110.53
1	B	288	ILE	N-CA-C	5.25	115.62	107.28
1	C	189	THR	N-CA-C	5.21	117.40	108.90
3	M	180	THR	N-CA-C	5.21	117.25	108.96
2	J	108	THR	CA-C-N	-5.20	115.72	122.94
2	J	108	THR	C-N-CA	-5.20	115.72	122.94
1	A	366	PHE	N-CA-C	5.17	116.73	108.41
1	A	143	GLY	N-CA-C	-5.16	104.06	112.83
2	K	120	SER	N-CA-C	5.16	116.93	108.52
3	L	97	THR	N-CA-C	5.15	117.99	109.85
5	E	83	ILE	CB-CA-C	-5.15	102.84	111.29
2	J	18	LEU	CA-C-N	-5.14	114.99	122.65
2	J	18	LEU	C-N-CA	-5.14	114.99	122.65
2	J	194	TYR	N-CA-C	5.14	117.98	109.46
1	C	56	VAL	N-CA-C	5.12	114.95	107.37
1	A	85	LYS	N-CA-C	-5.11	105.71	111.28
3	M	106	ILE	CA-C-N	5.11	129.19	122.30
3	M	106	ILE	C-N-CA	5.11	129.19	122.30
2	K	144	ASP	N-CA-C	5.10	116.88	110.91
2	K	83	ASP	CA-C-N	-5.10	114.83	119.82
2	K	83	ASP	C-N-CA	-5.10	114.83	119.82
2	J	83	ASP	CA-C-N	-5.09	114.83	119.82
2	J	83	ASP	C-N-CA	-5.09	114.83	119.82
1	C	176	LYS	N-CA-C	5.09	116.71	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	96	LEU	N-CA-C	-5.08	102.76	110.28
3	L	104	VAL	N-CA-C	5.08	116.61	108.89
4	H	195	ILE	CA-C-N	-5.07	115.46	122.30
4	H	195	ILE	C-N-CA	-5.07	115.46	122.30
1	C	144	VAL	N-CA-C	5.05	116.62	108.85
2	J	23	THR	N-CA-C	-5.03	101.67	109.72
1	C	73	ASP	N-CA-C	-5.03	101.50	109.59
4	H	201	LYS	N-CA-C	5.01	120.89	109.81
1	A	189	THR	N-CA-C	5.00	117.06	108.90
3	L	139	PHE	N-CA-C	5.00	117.02	109.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	78	LEU	Mainchain

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	3482	0	3526	111	0
1	B	3482	0	3526	105	0
1	C	3482	0	3526	117	0
2	J	1626	0	1610	56	0
2	K	1626	0	1610	63	0
2	N	1626	0	1610	37	0
3	L	1611	0	1564	45	1
3	M	1611	0	1564	52	0
3	O	1611	0	1564	20	1
4	D	1636	0	1579	28	0
4	F	1636	0	1579	32	0
4	H	1635	0	1576	34	0
5	E	1642	0	1597	34	0
5	G	1642	0	1597	21	0
5	I	1642	0	1597	31	0
All	All	29990	0	29625	709	1

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 12.

All (709) 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:B:374:THR:HG21	1:C:454:ASN:H	1.33	0.93
1:B:28:ILE:HA	1:B:43:GLY:HA3	1.53	0.90
5:E:106:ILE:O	5:E:166:GLN:NE2	2.04	0.89
3:L:12:SER:O	3:L:107:LYS:NZ	2.06	0.89
3:M:13:ALA:H	3:M:107:LYS:HZ3	1.11	0.89
4:H:75:LYS:NZ	3:M:77:SER:OG	2.05	0.88
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.55	0.87
4:H:195:ILE:HD11	4:H:208:ASP:HB3	1.56	0.87
1:C:407:ILE:HD11	1:C:457:TYR:HB3	1.56	0.86
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.56	0.86
1:B:267:THR:OG1	1:B:270:GLN:NE2	2.10	0.84
1:B:425:SER:HB2	1:B:449:THR:HG22	1.59	0.84
1:A:407:ILE:HD11	1:A:457:TYR:HB3	1.60	0.83
1:A:49:ARG:O	1:A:51:GLY:N	2.10	0.83
1:A:139:GLY:HA3	1:A:354:GLN:HE21	1.44	0.82
1:C:49:ARG:O	1:C:51:GLY:N	2.11	0.82
1:B:49:ARG:O	1:B:51:GLY:N	2.12	0.82
5:E:13:ALA:O	5:E:107:LYS:N	2.12	0.81
2:K:4:LEU:HD23	2:K:24:PHE:HB3	1.61	0.81
4:H:198:VAL:HB	4:H:207:VAL:HB	1.62	0.80
1:B:146:SER:H	1:C:407:ILE:HD12	1.47	0.80
5:E:106:ILE:N	5:E:166:GLN:OE1	2.14	0.79
1:A:28:ILE:HA	1:A:43:GLY:HA3	1.64	0.79
1:C:261:ILE:HA	1:C:264:MET:HE2	1.65	0.79
1:B:161:GLU:HG2	4:D:27:PHE:HA	1.63	0.79
1:C:28:ILE:HA	1:C:43:GLY:HA3	1.64	0.78
4:H:116:THR:HG23	4:H:147:PRO:HD3	1.65	0.78
1:A:454:ASN:H	1:C:374:THR:HG21	1.49	0.78
2:K:159:LEU:HD21	2:K:182:VAL:HG21	1.64	0.77
1:C:267:THR:OG1	1:C:270:GLN:NE2	2.16	0.77
1:B:261:ILE:HA	1:B:264:MET:HE2	1.67	0.76
4:D:181:VAL:HG11	5:E:135:LEU:HD22	1.68	0.76
3:M:108:ARG:HG3	3:M:109:THR:H	1.51	0.76
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.67	0.75
2:J:126:PRO:HG3	2:J:138:LEU:HB3	1.69	0.75
3:M:13:ALA:H	3:M:107:LYS:HG2	1.52	0.74
1:A:267:THR:OG1	1:A:270:GLN:NE2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:107:LYS:HD3	3:M:140:TYR:OH	1.86	0.74
1:C:161:GLU:HG2	4:H:27:PHE:HA	1.69	0.74
4:H:126:PRO:HG2	4:H:213:PRO:HG3	1.68	0.74
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.69	0.74
2:N:61:PRO:HD2	3:O:95:PRO:HG3	1.70	0.72
2:N:4:LEU:HD23	2:N:24:PHE:HB3	1.72	0.72
1:B:270:GLN:HG2	1:B:309:ILE:HD12	1.72	0.71
5:G:120:PRO:HD3	5:G:132:VAL:HG22	1.72	0.71
2:N:126:PRO:HG3	2:N:138:LEU:HB3	1.69	0.71
3:L:12:SER:HB3	3:L:107:LYS:HG3	1.71	0.71
1:C:252:LEU:HD22	1:C:301:VAL:HG21	1.73	0.71
3:M:13:ALA:N	3:M:107:LYS:HZ3	1.88	0.70
1:A:432:ILE:HD11	1:A:447:VAL:HG22	1.73	0.70
2:J:4:LEU:HD23	2:J:24:PHE:HB3	1.72	0.70
1:C:318:THR:O	1:C:339:ARG:NH2	2.24	0.70
3:M:211:ARG:HB3	3:M:211:ARG:HH11	1.55	0.70
3:M:211:ARG:HB3	3:M:211:ARG:NH1	2.06	0.69
1:B:217:ILE:HD13	1:C:218:GLU:HG3	1.75	0.69
4:F:181:VAL:HG11	5:G:135:LEU:HD22	1.74	0.69
5:E:19:VAL:HG21	5:E:78:LEU:HD22	1.73	0.69
2:K:143:LYS:NZ	3:M:129:THR:HG21	2.09	0.68
5:G:49:HIS:ND1	5:G:55:GLU:OE2	2.20	0.68
2:K:99:ASN:HB2	2:K:100(A):TYR:CE2	2.28	0.68
3:M:144:ALA:HB2	3:M:198:HIS:HD2	1.58	0.68
4:F:209:LYS:NZ	5:G:123:GLU:OE1	2.24	0.68
2:K:163:VAL:HG22	2:K:182:VAL:HB	1.76	0.68
1:A:239:VAL:HG13	1:B:246:PRO:HG2	1.75	0.68
1:B:444:ASN:ND2	1:B:462:GLN:O	2.27	0.67
2:J:39:GLN:HB2	2:J:45:LEU:HD23	1.77	0.67
2:J:143:LYS:NZ	3:L:129:THR:HG21	2.10	0.67
1:B:48:LEU:HB2	1:B:308:VAL:HB	1.75	0.67
1:A:261:ILE:HA	1:A:264:MET:HE2	1.77	0.66
1:A:444:ASN:ND2	1:A:462:GLN:O	2.28	0.66
1:C:425:SER:HB2	1:C:449:THR:HG22	1.77	0.66
1:A:146:SER:H	1:B:407:ILE:HD12	1.59	0.66
1:A:246:PRO:HG2	1:C:239:VAL:HG13	1.76	0.66
2:K:119:PRO:HB3	2:K:145:TYR:HB3	1.75	0.66
2:K:126:PRO:HG3	2:K:138:LEU:HB3	1.78	0.66
1:C:146:SER:HB3	1:C:149:ALA:HB2	1.76	0.66
2:J:171:GLN:HA	3:L:160:GLN:HE22	1.61	0.66
5:E:107:LYS:HG2	5:E:109:THR:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ILE:HD11	1:B:199:ILE:HG21	1.78	0.66
3:L:105:GLU:CD	3:L:106:ILE:H	2.03	0.65
1:B:432:ILE:HD11	1:B:447:VAL:HG22	1.76	0.65
2:J:163:VAL:HG22	2:J:182:VAL:HB	1.78	0.65
5:E:105:GLU:HG2	5:E:166:GLN:OE1	1.96	0.65
1:B:407:ILE:HD11	1:B:457:TYR:HB3	1.78	0.65
4:F:123:PRO:HD3	4:F:209:LYS:HE2	1.79	0.65
4:D:12:VAL:HG21	4:D:18:LEU:HB2	1.79	0.65
1:B:332:ILE:HG22	1:B:475:ILE:HD11	1.78	0.65
5:E:166:GLN:NE2	5:E:171:SER:O	2.28	0.65
1:B:56:VAL:HG22	1:B:300:VAL:HG22	1.78	0.64
1:B:442:VAL:HG11	1:B:447:VAL:HG21	1.78	0.64
3:M:13:ALA:N	3:M:107:LYS:HG2	2.12	0.64
4:H:82:MET:HB3	4:H:82(C):LEU:HD21	1.78	0.64
1:A:64:ILE:HD11	1:A:199:ILE:HG21	1.78	0.64
4:H:31:HIS:HB3	4:H:98:VAL:HG13	1.79	0.64
1:B:429:ARG:HH11	1:B:432:ILE:HG22	1.63	0.63
1:C:177:ALA:O	1:C:189:THR:OG1	2.15	0.63
3:M:151:ASP:OD2	3:M:189:HIS:ND1	2.30	0.63
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.79	0.63
1:C:203:LEU:O	1:C:206:ILE:HG22	1.99	0.63
4:H:119:PRO:HB3	4:H:145:TYR:HB3	1.80	0.63
5:I:36:TYR:HE1	5:I:89:GLN:HG2	1.63	0.63
5:E:108:ARG:HH11	5:E:108:ARG:HG3	1.62	0.63
1:C:499:ILE:O	1:C:503:LEU:N	2.32	0.63
2:K:143:LYS:HZ1	3:M:129:THR:HG21	1.64	0.63
1:A:445:LYS:HZ3	1:A:463:GLU:HA	1.64	0.62
1:A:402:VAL:HG11	1:C:373:LEU:HD13	1.81	0.62
3:L:2:ILE:O	3:L:97:THR:HG21	1.98	0.62
1:C:432:ILE:HD11	1:C:447:VAL:HG22	1.80	0.62
4:H:5:VAL:HG23	4:H:23:ALA:HB3	1.80	0.62
2:N:99:ASN:HB2	2:N:100(A):TYR:CE2	2.35	0.62
1:B:96:LEU:HD13	1:C:279:GLN:HG2	1.80	0.62
2:K:100(A):TYR:HB3	3:M:34:HIS:ND1	2.14	0.62
1:A:150:SER:OG	1:A:302:GLN:OE1	2.17	0.62
1:B:209:LYS:O	1:B:211:SER:N	2.31	0.62
3:L:14:SER:OG	3:L:107:LYS:O	2.15	0.62
1:C:62:SER:HB3	1:C:196:LYS:HA	1.80	0.62
5:E:120:PRO:HD3	5:E:132:VAL:HG22	1.82	0.62
1:A:75:LYS:HB2	1:A:214:ILE:HG21	1.81	0.62
1:A:259:SER:HA	2:K:53:TRP:HZ2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:82:MET:HB3	4:D:82(C):LEU:HD21	1.82	0.62
2:J:168:ALA:HB2	2:J:178:LEU:HD23	1.82	0.61
1:A:209:LYS:O	1:A:211:SER:N	2.33	0.61
4:H:117:LYS:HD3	4:H:175:LEU:HD21	1.82	0.61
3:L:29:ARG:HG3	3:L:68:GLY:HA2	1.81	0.61
3:M:8:PRO:HG2	3:M:11:LEU:HD13	1.83	0.61
3:M:13:ALA:H	3:M:107:LYS:NZ	1.93	0.61
1:C:487:GLU:OE1	1:C:498:LYS:NZ	2.33	0.61
5:E:108:ARG:O	5:E:109:THR:OG1	2.10	0.61
1:C:332:ILE:HG22	1:C:475:ILE:HD11	1.83	0.60
1:A:182:SER:O	4:F:97:ILE:HA	2.00	0.60
2:J:22:CYS:HB2	2:J:36:TRP:CZ2	2.35	0.60
1:A:332:ILE:HG22	1:A:475:ILE:HD11	1.82	0.60
2:J:123:PRO:HG3	2:J:209:LYS:HG2	1.83	0.60
1:C:49:ARG:O	1:C:49:ARG:HG2	2.01	0.60
4:F:31:HIS:HB3	4:F:98:VAL:HG13	1.83	0.60
1:B:31:GLU:HG2	1:B:467:LEU:HD23	1.84	0.60
4:D:94:ARG:NH2	4:D:101:ASP:OD2	2.33	0.60
2:N:30:SER:HB3	2:N:73:THR:HG21	1.83	0.60
2:K:124:LEU:HB3	3:M:118:PHE:CD2	2.37	0.60
2:N:135:THR:N	2:N:186:SER:HG	2.00	0.60
1:C:322:CYS:HA	1:C:475:ILE:HD13	1.84	0.59
1:C:310:ASP:H	1:C:364:ARG:HH22	1.50	0.59
1:C:195:LEU:HD21	1:C:226:LYS:HB3	1.85	0.59
1:C:408:THR:O	1:C:460:ASN:ND2	2.36	0.59
5:I:197:THR:HG22	5:I:204:PRO:HB3	1.85	0.59
4:H:200:HIS:CE1	4:H:202:PRO:HG2	2.37	0.59
1:B:499:ILE:O	1:B:503:LEU:N	2.36	0.59
3:L:189:HIS:O	3:L:211:ARG:NH1	2.36	0.59
1:B:49:ARG:O	1:B:49:ARG:HG2	2.03	0.59
2:K:84:PRO:HA	2:K:111:VAL:HB	1.85	0.58
3:L:105:GLU:CD	3:L:166:GLN:HE22	2.10	0.58
1:A:338:ASP:HB2	1:A:342:TYR:OH	2.04	0.58
2:J:30:SER:HB3	2:J:73:THR:HG21	1.84	0.58
5:E:107:LYS:HG3	5:E:140:TYR:CE1	2.39	0.58
4:F:12:VAL:HG21	4:F:18:LEU:HB2	1.86	0.58
2:J:143:LYS:HZ1	3:L:129:THR:HG21	1.68	0.58
3:M:11:LEU:HB3	3:M:104:VAL:HG22	1.86	0.58
4:H:112:SER:HB3	4:H:146:PHE:CZ	2.38	0.58
2:J:35:SER:HB2	2:J:52:TRP:CE3	2.39	0.57
5:G:151:ASP:HA	5:G:191:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:89:THR:HA	2:K:108:THR:HA	1.85	0.57
1:A:75:LYS:HE2	1:B:218:GLU:OE2	2.04	0.57
1:B:408:THR:O	1:B:460:ASN:ND2	2.37	0.57
1:A:442:VAL:HG11	1:A:447:VAL:HG21	1.86	0.57
1:B:146:SER:N	1:C:407:ILE:HD12	2.18	0.57
2:N:40:PRO:HB2	2:N:43:LYS:HD2	1.85	0.57
1:A:161:GLU:OE1	4:F:28:SER:OG	2.18	0.57
2:J:188:SER:O	2:J:192:GLN:HB3	2.04	0.57
1:C:193:LEU:HD13	1:C:195:LEU:HG	1.85	0.57
5:I:7:SER:OG	5:I:8:PRO:HA	2.03	0.57
2:J:159:LEU:HD21	2:J:182:VAL:HG21	1.86	0.57
1:C:445:LYS:NZ	1:C:463:GLU:HA	2.20	0.57
1:C:165:ASN:ND2	1:C:294:GLU:OE2	2.32	0.57
3:L:13:ALA:N	3:L:107:LYS:H	2.03	0.57
4:D:200:HIS:CE1	4:D:202:PRO:HG2	2.40	0.57
3:L:211:ARG:HH11	3:L:211:ARG:HB3	1.70	0.56
2:K:123:PRO:HG3	2:K:209:LYS:HG2	1.85	0.56
1:A:240:ASN:HB3	1:A:243:VAL:O	2.06	0.56
1:C:48:LEU:HB2	1:C:308:VAL:HB	1.86	0.56
1:C:429:ARG:HH11	1:C:432:ILE:HG22	1.70	0.56
1:C:445:LYS:HZ3	1:C:463:GLU:HA	1.70	0.56
2:N:22:CYS:HB2	2:N:36:TRP:CZ2	2.41	0.56
3:O:1:ASP:HB2	3:O:95:PRO:HD2	1.87	0.56
5:E:106:ILE:HG22	5:E:171:SER:HB3	1.88	0.56
3:L:211:ARG:NH1	3:L:211:ARG:HB3	2.21	0.56
1:A:270:GLN:HG2	1:A:309:ILE:HD12	1.87	0.56
5:E:3:GLN:HB2	5:E:26:SER:HB3	1.88	0.56
1:B:162:GLY:O	1:B:166:LYS:HG3	2.06	0.56
1:B:423:THR:HG23	1:B:431:ILE:HG23	1.87	0.56
2:K:141:LEU:HD13	2:K:179:SER:OG	2.05	0.56
1:A:49:ARG:O	1:A:49:ARG:HG2	2.05	0.56
2:J:100(A):TYR:HB3	3:L:34:HIS:ND1	2.21	0.56
1:B:96:LEU:HB3	1:B:97:MET:HE2	1.88	0.56
2:J:137:ALA:HB2	2:J:183:THR:HG22	1.88	0.55
5:G:30:LYS:HD2	5:G:32:TYR:CE2	2.40	0.55
1:B:150:SER:OG	1:B:302:GLN:OE1	2.23	0.55
1:B:232:GLU:HG2	1:B:250:TYR:CE2	2.41	0.55
3:L:158:ASN:O	3:L:179:LEU:HD12	2.07	0.55
2:N:96:MET:HB2	2:N:99:ASN:OD1	2.06	0.55
1:A:48:LEU:HB2	1:A:308:VAL:HB	1.87	0.55
4:F:200:HIS:HB3	4:F:205:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4:LEU:HD23	2:J:24:PHE:CB	2.36	0.55
1:A:74:ALA:O	1:A:77:LYS:HG2	2.07	0.55
1:B:75:LYS:HB2	1:B:214:ILE:HG21	1.88	0.55
2:K:30:SER:HB3	2:K:73:THR:HG21	1.89	0.55
1:A:325:ASN:ND2	1:A:331:ASN:OD1	2.40	0.55
1:C:423:THR:HG23	1:C:431:ILE:HG23	1.88	0.55
3:L:12:SER:OG	3:L:106:ILE:N	2.40	0.55
1:B:338:ASP:HB2	1:B:342:TYR:OH	2.07	0.55
2:J:6:GLU:N	2:J:6:GLU:OE1	2.39	0.55
4:D:195:ILE:HD11	4:D:208:ASP:HB3	1.89	0.55
1:C:407:ILE:HD13	1:C:458:TYR:O	2.07	0.54
5:E:30:LYS:HD2	5:E:32:TYR:CE2	2.42	0.54
5:I:12:SER:OG	5:I:105:GLU:OE1	2.21	0.54
1:B:217:ILE:HG13	1:B:217:ILE:O	2.07	0.54
3:L:15:VAL:HA	3:L:78:LEU:O	2.07	0.54
1:B:146:SER:HB3	1:B:149:ALA:HB2	1.88	0.54
1:A:35:SER:O	1:A:474:ILE:HG12	2.08	0.54
2:K:144:ASP:OD1	2:K:171:GLN:NE2	2.26	0.54
2:N:61:PRO:CD	3:O:95:PRO:HG3	2.38	0.54
4:H:123:PRO:HB3	4:H:211:VAL:HG22	1.90	0.54
5:E:166:GLN:HE21	5:E:171:SER:C	2.15	0.54
4:H:74:SER:O	3:M:60:SER:OG	2.25	0.54
5:I:105:GLU:HG3	5:I:173:TYR:OH	2.08	0.54
5:E:108:ARG:O	5:E:108:ARG:NH1	2.41	0.54
1:C:262:ASN:ND2	2:J:97:ILE:HD12	2.23	0.54
1:A:95:LEU:HD21	1:B:275:SER:O	2.08	0.53
1:A:247:VAL:HG22	1:A:287:SER:HB2	1.89	0.53
1:B:177:ALA:O	1:B:189:THR:OG1	2.26	0.53
1:C:279:GLN:CD	1:C:279:GLN:H	2.16	0.53
2:J:124:LEU:HB3	3:L:118:PHE:CD2	2.43	0.53
2:J:99:ASN:HB2	2:J:100(A):TYR:CE2	2.44	0.53
4:F:163:VAL:HG22	4:F:182:VAL:HG22	1.88	0.53
3:M:66:GLY:HA3	3:M:71:PHE:HA	1.89	0.53
1:A:425:SER:HB2	1:A:449:THR:HG22	1.88	0.53
1:B:163:GLU:HG3	1:B:181:LEU:HD22	1.90	0.53
1:B:279:GLN:CD	1:B:279:GLN:H	2.16	0.53
2:K:35:SER:HB2	2:K:52:TRP:CE3	2.43	0.53
2:N:159:LEU:HD21	2:N:182:VAL:HG21	1.91	0.53
1:A:236:GLU:OE2	1:A:248:SER:OG	2.20	0.53
1:A:423:THR:HG23	1:A:431:ILE:HG23	1.90	0.53
1:B:49:ARG:HE	1:B:368:ASP:CG	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3:THR:OG1	2:K:25:SER:OG	2.25	0.53
2:N:168:ALA:HB2	2:N:178:LEU:HD23	1.90	0.53
3:M:30:VAL:HG13	3:M:92:SER:OG	2.08	0.52
3:O:8:PRO:HB2	3:O:10:THR:O	2.09	0.52
1:A:407:ILE:HD13	1:A:458:TYR:O	2.10	0.52
1:B:161:GLU:OE1	1:B:162:GLY:N	2.43	0.52
1:C:232:GLU:HG2	1:C:250:TYR:CE2	2.44	0.52
3:L:13:ALA:CA	3:L:107:LYS:H	2.23	0.52
5:I:91:TYR:HA	5:I:96:LEU:HD22	1.92	0.52
5:I:120:PRO:HD3	5:I:132:VAL:HG22	1.92	0.52
2:K:123:PRO:HG3	2:K:209:LYS:CG	2.39	0.52
1:B:252:LEU:HD21	1:B:260:LEU:HD12	1.90	0.52
1:C:324:THR:HG21	1:C:437:ASN:O	2.09	0.52
3:M:8:PRO:HB2	3:M:10:THR:O	2.10	0.52
1:A:178:VAL:HG12	1:A:188:LEU:HD12	1.91	0.52
1:C:262:ASN:O	2:J:56:LYS:NZ	2.35	0.52
5:E:91:TYR:HA	5:E:96:LEU:HD22	1.92	0.52
3:L:124:GLN:HG2	3:L:129:THR:O	2.09	0.52
4:F:29:PHE:CD2	4:F:76:ASN:HA	2.45	0.52
2:J:35:SER:HB3	2:J:95:ASP:HB3	1.92	0.51
5:I:108:ARG:O	5:I:109:THR:OG1	2.20	0.51
2:K:6:GLU:N	2:K:6:GLU:OE1	2.42	0.51
2:K:123:PRO:HA	2:K:140:CYS:HA	1.91	0.51
3:O:33:MET:C	3:O:34:HIS:HD2	2.18	0.51
2:N:153:SER:OG	2:N:197:ASN:HB2	2.09	0.51
1:C:56:VAL:HG22	1:C:300:VAL:HG22	1.92	0.51
4:H:181:VAL:HG11	5:I:135:LEU:HD22	1.92	0.51
1:A:67:ASN:H	1:A:67:ASN:HD22	1.57	0.51
1:C:49:ARG:HE	1:C:368:ASP:CG	2.18	0.51
4:D:13:GLN:HB2	4:D:16:ARG:HD2	1.91	0.51
1:A:329:GLY:C	1:A:331:ASN:H	2.18	0.51
2:J:123:PRO:HG3	2:J:209:LYS:CG	2.40	0.51
5:I:108:ARG:HG3	5:I:171:SER:HB2	1.92	0.51
1:C:35:SER:O	1:C:474:ILE:HG12	2.11	0.51
4:H:143:LYS:HE2	5:I:129:THR:HG21	1.93	0.51
1:B:178:VAL:HG12	1:B:188:LEU:HD12	1.93	0.50
4:D:31:HIS:HB3	4:D:98:VAL:HG13	1.93	0.50
3:M:89:PHE:CE1	3:M:96:PHE:HB3	2.46	0.50
4:F:94:ARG:NH2	4:F:101:ASP:OD2	2.44	0.50
2:K:39:GLN:HB2	2:K:45:LEU:HD23	1.92	0.50
1:A:92:GLU:HG2	1:B:254:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD13	1:A:191:LYS:HB2	1.93	0.50
1:B:165:ASN:ND2	1:B:294:GLU:OE2	2.37	0.50
2:J:40:PRO:HB2	2:J:43:LYS:HD2	1.92	0.50
2:K:12:VAL:HG13	2:K:111:VAL:HG22	1.94	0.50
2:J:64:LYS:HD2	2:J:65:ASP:HA	1.93	0.50
2:J:99:ASN:HB2	2:J:100(A):TYR:CZ	2.47	0.50
1:A:225:GLN:OE1	1:C:81:GLN:NE2	2.45	0.50
2:N:35:SER:HB2	2:N:52:TRP:CE3	2.46	0.50
1:A:499:ILE:O	1:A:503:LEU:N	2.44	0.50
5:I:108:ARG:NH1	5:I:111:ALA:HB2	2.27	0.50
2:K:126:PRO:HD2	2:K:213:PRO:HA	1.92	0.50
3:M:52:SER:HA	3:M:64:GLY:HA3	1.93	0.50
1:A:67:ASN:HD22	1:A:67:ASN:N	2.09	0.50
2:K:51:ILE:HD13	2:K:71:LYS:HB3	1.94	0.50
3:M:12:SER:HB3	3:M:107:LYS:HD2	1.94	0.50
1:B:505:PHE:O	1:B:505:PHE:HD1	1.95	0.49
1:B:500:ASN:O	1:B:504:ALA:N	2.40	0.49
1:C:162:GLY:O	1:C:166:LYS:HG3	2.12	0.49
1:B:53:TYR:CD2	1:B:264:MET:HG2	2.47	0.49
5:G:34:ASN:HB2	5:G:89:GLN:HG2	1.94	0.49
5:G:36:TYR:HE1	5:G:89:GLN:HG2	1.76	0.49
5:I:30:LYS:HD2	5:I:32:TYR:CE2	2.47	0.49
2:K:124:LEU:N	2:K:139:GLY:O	2.38	0.49
1:A:162:GLY:O	1:A:166:LYS:HG3	2.12	0.49
2:J:64:LYS:CD	2:J:65:ASP:HA	2.42	0.49
1:A:79:ILE:HD12	1:A:214:ILE:HD11	1.95	0.49
1:C:262:ASN:HD21	2:J:97:ILE:HD12	1.77	0.49
2:J:195:ILE:HG22	2:J:197:ASN:HD22	1.78	0.49
1:A:272:LYS:NZ	2:K:99:ASN:HA	2.27	0.49
2:J:33:GLY:HA2	2:J:97:ILE:HG22	1.95	0.49
1:A:429:ARG:NE	5:I:93:ASN:OD1	2.45	0.49
2:K:138:LEU:HD13	2:K:211:VAL:HG11	1.93	0.49
1:B:67:ASN:HD22	1:B:67:ASN:H	1.58	0.49
2:N:170:LEU:HD13	2:N:176:TYR:CE1	2.47	0.49
4:H:198:VAL:N	4:H:207:VAL:O	2.34	0.49
5:E:83:ILE:HD11	5:E:168:SER:OG	2.12	0.49
2:K:100(A):TYR:HD2	3:M:34:HIS:CE1	2.31	0.49
2:N:59:TYR:OH	2:N:69:ILE:HG22	2.13	0.49
1:B:62:SER:HB3	1:B:196:LYS:HA	1.95	0.48
2:K:35:SER:HB2	2:K:52:TRP:CD2	2.48	0.48
3:M:105:GLU:HB3	3:M:107:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:100(A):TYR:HD2	3:O:34:HIS:CE1	2.31	0.48
2:N:171:GLN:HA	3:O:160:GLN:HE22	1.78	0.48
1:B:75:LYS:NZ	1:B:215:SER:O	2.38	0.48
5:G:37:HIS:HB2	5:G:47:LEU:HD11	1.95	0.48
3:M:124:GLN:HE22	3:M:131:SER:CB	2.27	0.48
1:C:188:LEU:HD21	1:C:263:ASP:HB2	1.95	0.48
1:C:505:PHE:HD1	1:C:505:PHE:O	1.96	0.48
4:D:41:PRO:HG2	4:D:148:GLU:OE2	2.12	0.48
1:A:30:GLU:O	1:A:466:SER:HA	2.13	0.48
1:A:62:SER:HB3	1:A:196:LYS:HA	1.95	0.48
1:A:445:LYS:NZ	1:A:463:GLU:HA	2.28	0.48
1:A:462:GLN:HA	1:C:156:LYS:HE2	1.94	0.48
1:C:93:LEU:HD22	1:C:289:MET:SD	2.53	0.48
1:C:139:GLY:HA3	1:C:354:GLN:HE21	1.79	0.48
3:M:108:ARG:HG3	3:M:109:THR:N	2.25	0.48
3:M:158:ASN:O	3:M:179:LEU:HD12	2.14	0.48
5:I:136:LEU:HB2	5:I:175:LEU:HB3	1.96	0.48
1:A:454:ASN:HD21	1:C:346:ALA:HB3	1.79	0.48
4:F:184:VAL:HG11	4:F:194:TYR:CE1	2.47	0.48
2:K:137:ALA:HB2	2:K:183:THR:HG22	1.96	0.48
3:M:33:MET:C	3:M:34:HIS:HD2	2.21	0.48
2:J:199:ASN:OD1	2:J:206:LYS:HG2	2.14	0.48
4:H:123:PRO:HD3	4:H:209:LYS:HE2	1.95	0.48
5:E:10:SER:HA	5:E:103:LYS:O	2.13	0.48
2:J:195:ILE:HG22	2:J:197:ASN:ND2	2.28	0.48
4:H:2:VAL:N	4:H:26:GLY:HA3	2.29	0.48
5:I:54:LEU:HD21	5:I:62:PHE:O	2.14	0.48
3:L:33:MET:C	3:L:34:HIS:HD2	2.22	0.48
4:D:60:ALA:O	4:D:64:LYS:HG3	2.14	0.48
3:O:140:TYR:CG	3:O:141:PRO:HA	2.48	0.48
1:C:94:GLN:HA	1:C:292:ILE:HD11	1.96	0.47
2:K:122:PHE:CG	3:M:124:GLN:HB2	2.49	0.47
1:A:96:LEU:HD13	1:B:279:GLN:HG2	1.95	0.47
5:G:158:ASN:O	5:G:179:LEU:HD12	2.14	0.47
2:K:171:GLN:N	2:K:175:LEU:O	2.45	0.47
4:H:152:VAL:HA	4:H:197:ASN:O	2.13	0.47
2:N:135:THR:N	2:N:186:SER:OG	2.48	0.47
1:A:138:LEU:O	1:A:354:GLN:NE2	2.48	0.47
1:A:217:ILE:HG13	1:A:220:VAL:HG22	1.97	0.47
4:H:152:VAL:HG22	4:H:198:VAL:HA	1.96	0.47
2:K:99:ASN:HB2	2:K:100(A):TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:148:TRP:CE2	3:O:179:LEU:HB2	2.50	0.47
1:A:177:ALA:O	1:A:189:THR:OG1	2.32	0.47
1:C:67:ASN:CB	1:C:207:LEU:HD23	2.44	0.47
1:C:252:LEU:HD21	1:C:260:LEU:HD12	1.96	0.47
3:L:107:LYS:HA	3:L:108:ARG:HA	1.67	0.47
5:G:105:GLU:HG2	5:G:166:GLN:OE1	2.15	0.47
1:A:88:ASN:O	1:A:92:GLU:HG3	2.14	0.47
1:B:292:ILE:HG22	1:B:297:LEU:HA	1.97	0.47
2:J:84:PRO:HA	2:J:111:VAL:HB	1.96	0.47
1:A:218:GLU:OE1	1:A:218:GLU:N	2.41	0.47
1:B:216:ASN:HB2	1:B:218:GLU:OE1	2.15	0.47
1:B:445:LYS:HZ3	1:B:463:GLU:HA	1.79	0.47
1:C:429:ARG:O	5:E:32:TYR:OH	2.32	0.47
4:F:119:PRO:HB3	4:F:145:TYR:HB3	1.95	0.47
5:G:105:GLU:HG3	5:G:173:TYR:OH	2.14	0.47
5:E:140:TYR:CG	5:E:141:PRO:HA	2.50	0.47
1:A:163:GLU:HG3	1:A:181:LEU:HD22	1.96	0.47
2:J:124:LEU:HB2	2:J:139:GLY:O	2.15	0.47
5:I:37:HIS:HB2	5:I:47:LEU:HD11	1.97	0.47
2:N:15:THR:HA	2:N:82(B):ASN:HA	1.97	0.47
3:O:124:GLN:HG2	3:O:129:THR:O	2.15	0.47
3:L:114:SER:HB2	3:L:137:ASN:HB3	1.96	0.46
4:F:108:THR:HG21	4:F:149:PRO:HD3	1.98	0.46
5:G:107:LYS:HA	5:G:140:TYR:OH	2.15	0.46
1:A:329:GLY:C	1:A:331:ASN:N	2.74	0.46
3:L:13:ALA:HB3	3:L:78:LEU:HD22	1.96	0.46
4:H:11:VAL:HG21	4:H:146:PHE:HE2	1.81	0.46
4:D:82:MET:HE2	4:D:82(C):LEU:HD21	1.98	0.46
1:B:66:GLU:N	1:B:66:GLU:OE2	2.48	0.46
1:B:407:ILE:HD13	1:B:458:TYR:O	2.15	0.46
3:L:8:PRO:HG2	3:L:11:LEU:HD22	1.98	0.46
5:E:105:GLU:HG2	5:E:166:GLN:CD	2.40	0.46
3:M:105:GLU:HG2	3:M:106:ILE:N	2.30	0.46
2:N:35:SER:HB2	2:N:52:TRP:CD2	2.50	0.46
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.69	0.46
1:B:318:THR:O	1:B:339:ARG:NH2	2.47	0.46
3:M:48:ILE:HG13	3:M:73:LEU:HD13	1.98	0.46
1:A:264:MET:HE1	1:A:274:MET:SD	2.55	0.46
1:B:218:GLU:OE1	1:B:218:GLU:N	2.38	0.46
1:C:183:ASN:HD21	1:C:185:VAL:HB	1.80	0.46
3:M:148:TRP:NE1	3:M:177:SER:OG	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:36:TRP:C	2:N:37:ILE:HG13	2.41	0.46
1:A:289:MET:HE1	1:A:292:ILE:HG23	1.97	0.46
1:B:67:ASN:HD22	1:B:67:ASN:N	2.12	0.46
1:C:488:PHE:CD1	1:C:488:PHE:N	2.84	0.46
4:F:193:THR:HG23	4:F:210:LYS:NZ	2.30	0.46
5:I:89:GLN:HE21	5:I:89:GLN:HB2	1.57	0.46
5:I:93:ASN:HB3	5:I:94:LEU:H	1.43	0.46
4:D:193:THR:HG23	4:D:210:LYS:NZ	2.31	0.46
1:A:56:VAL:HG23	1:A:187:VAL:HG21	1.96	0.46
1:B:176:LYS:HE3	1:B:190:PHE:CZ	2.51	0.46
1:C:139:GLY:HA3	1:C:354:GLN:NE2	2.30	0.46
2:J:89:THR:HA	2:J:108:THR:HA	1.97	0.46
1:A:270:GLN:HG2	1:A:309:ILE:CD1	2.45	0.46
1:C:68:LYS:HA	1:C:68:LYS:HD3	1.70	0.46
1:C:270:GLN:HG2	1:C:309:ILE:HD12	1.97	0.46
2:J:13:LYS:HA	2:J:14:PRO:HD3	1.82	0.46
2:J:36:TRP:C	2:J:37:ILE:HG13	2.41	0.46
2:K:119:PRO:HG3	2:K:200:HIS:ND1	2.30	0.46
1:A:250:TYR:CE2	1:C:235:ARG:HD2	2.50	0.46
1:B:221:ILE:O	1:B:224:GLN:HG2	2.16	0.46
2:K:122:PHE:CE2	3:M:124:GLN:HG3	2.51	0.46
3:O:211:ARG:HH11	3:O:211:ARG:HB3	1.81	0.46
4:F:159:LEU:HD21	4:F:182:VAL:HG11	1.97	0.45
4:H:31:HIS:O	4:H:98:VAL:HG13	2.16	0.45
3:M:105:GLU:O	3:M:107:LYS:NZ	2.48	0.45
1:C:442:VAL:HG11	1:C:447:VAL:HG21	1.98	0.45
3:L:140:TYR:CG	3:L:141:PRO:HA	2.50	0.45
3:L:151:ASP:HA	3:L:191:VAL:HG22	1.97	0.45
1:C:376:PRO:O	1:C:379:VAL:HG23	2.17	0.45
4:H:142:VAL:N	4:H:178:LEU:O	2.45	0.45
2:K:64:LYS:HD2	2:K:65:ASP:HA	1.98	0.45
2:K:100(A):TYR:CE2	3:M:49:TYR:HB2	2.51	0.45
1:C:73:ASP:HB3	1:C:76:VAL:HG23	1.99	0.45
3:L:124:GLN:HE22	3:L:131:SER:CB	2.29	0.45
2:K:154:TRP:HA	2:K:195:ILE:O	2.16	0.45
1:A:53:TYR:CD2	1:A:264:MET:HG2	2.52	0.45
1:A:345:ASN:OD1	1:A:346:ALA:N	2.50	0.45
2:J:13:LYS:O	2:J:16:GLN:HB2	2.17	0.45
4:H:112:SER:CB	4:H:146:PHE:CZ	2.99	0.45
1:B:94:GLN:HA	1:B:292:ILE:HD11	1.98	0.45
1:B:139:GLY:HA3	1:B:354:GLN:HE21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:LEU:CD2	1:C:226:LYS:HB3	2.46	0.45
1:C:272:LYS:HZ2	2:J:99:ASN:HA	1.81	0.45
2:N:125:ALA:HA	2:N:126:PRO:HD3	1.68	0.45
1:B:375:LEU:HA	1:B:376:PRO:HD3	1.84	0.45
3:L:13:ALA:O	3:L:106:ILE:HA	2.17	0.45
1:A:216:ASN:HB2	1:A:218:GLU:OE1	2.17	0.45
1:B:264:MET:HE1	1:B:274:MET:HE1	1.99	0.45
2:J:197:ASN:HB3	2:J:208:ASP:OD1	2.17	0.45
3:L:36:TYR:CZ	3:L:46:LEU:HD13	2.52	0.45
3:M:120:PRO:HD3	3:M:132:VAL:HG22	1.98	0.45
2:N:64:LYS:HD2	2:N:65:ASP:HA	1.99	0.45
1:C:161:GLU:CD	1:C:162:GLY:H	2.25	0.45
4:F:5:VAL:HG23	4:F:23:ALA:HB3	1.98	0.45
5:I:108:ARG:HG3	5:I:170:ASP:O	2.17	0.45
5:I:151:ASP:OD2	5:I:189:HIS:ND1	2.41	0.45
2:K:171:GLN:HE21	2:K:175:LEU:HB2	1.82	0.45
2:K:200:HIS:CD2	2:K:203:SER:H	2.35	0.45
3:O:61:ARG:NH1	3:O:82:ASP:OD1	2.50	0.45
1:A:176:LYS:HE3	1:A:190:PHE:CZ	2.52	0.45
4:F:193:THR:HG23	4:F:210:LYS:HZ2	1.82	0.45
4:F:200:HIS:CE1	4:F:202:PRO:HG2	2.52	0.45
5:E:19:VAL:CG2	5:E:78:LEU:HD22	2.45	0.45
1:B:156:LYS:HE2	1:C:462:GLN:HA	1.98	0.44
1:B:325:ASN:ND2	1:B:331:ASN:OD1	2.50	0.44
1:C:49:ARG:NH1	1:C:51:GLY:O	2.50	0.44
2:J:154:TRP:C	2:J:156:SER:H	2.25	0.44
2:K:4:LEU:HD23	2:K:24:PHE:CB	2.37	0.44
1:C:229:ARG:HH22	1:C:256:GLU:CD	2.24	0.44
2:J:4:LEU:HD13	2:J:93:ALA:HA	1.99	0.44
5:I:105:GLU:OE2	5:I:140:TYR:HE2	2.00	0.44
4:D:184:VAL:HG11	4:D:194:TYR:CE1	2.52	0.44
2:K:20:LEU:O	2:K:79:VAL:HA	2.18	0.44
2:K:200:HIS:HE2	2:K:202:PRO:HB2	1.82	0.44
1:A:259:SER:HA	2:K:53:TRP:CZ2	2.48	0.44
1:A:276:ASN:HD21	2:K:98:PHE:HB3	1.81	0.44
1:A:315:LYS:HB2	1:A:341:TRP:CH2	2.53	0.44
1:C:181:LEU:HA	1:C:181:LEU:HD23	1.59	0.44
1:C:267:THR:HG1	1:C:270:GLN:HE21	1.60	0.44
4:F:143:LYS:NZ	4:F:171:GLN:OE1	2.34	0.44
5:E:197:THR:HG22	5:E:204:PRO:HB3	1.99	0.44
1:C:56:VAL:HB	1:C:189:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:149:LYS:HA	3:L:153:ALA:O	2.17	0.44
5:G:89:GLN:HE21	5:G:89:GLN:HB2	1.59	0.44
5:G:118:PHE:HA	5:G:119:PRO:HD2	1.90	0.44
5:I:105:GLU:HG2	5:I:166:GLN:OE1	2.17	0.44
5:I:145:LYS:HB3	5:I:197:THR:OG1	2.17	0.44
4:D:100(C):TYR:O	5:E:91:TYR:HB2	2.17	0.44
5:E:93:ASN:HB3	5:E:94:LEU:H	1.45	0.44
5:G:145:LYS:HB3	5:G:197:THR:OG1	2.18	0.44
4:D:97:ILE:HD12	4:D:100(D):TYR:CD1	2.53	0.44
2:K:36:TRP:C	2:K:37:ILE:HG13	2.41	0.44
3:O:33:MET:C	3:O:34:HIS:CD2	2.94	0.44
5:I:158:ASN:O	5:I:179:LEU:HD12	2.18	0.44
2:K:38:ARG:HG2	2:K:48:LEU:HD11	1.98	0.44
1:B:267:THR:HG1	1:B:270:GLN:HE21	1.60	0.44
1:C:83:LEU:HD21	1:C:203:LEU:HD22	2.00	0.44
1:C:240:ASN:HB3	1:C:243:VAL:O	2.18	0.44
4:F:200:HIS:ND1	4:F:203:SER:OG	2.38	0.44
1:C:27:ASN:HD22	1:C:363:ASN:ND2	2.16	0.44
1:A:334:LEU:HD11	1:A:395:ILE:HD12	2.00	0.44
1:A:491:SER:O	1:A:495:VAL:HG23	2.18	0.44
1:B:264:MET:HE1	1:B:274:MET:SD	2.58	0.44
1:B:321:LEU:O	1:B:334:LEU:N	2.50	0.44
1:B:396:MET:HB2	1:B:487:GLU:O	2.18	0.44
1:B:488:PHE:HB2	1:C:488:PHE:CZ	2.53	0.44
1:C:67:ASN:HB2	1:C:207:LEU:HD23	1.99	0.44
2:J:117:LYS:O	2:J:203:SER:CB	2.66	0.44
4:D:82(C):LEU:HB3	4:D:111:VAL:HG21	2.00	0.44
5:E:138:ASN:HA	5:E:172:THR:HB	1.99	0.44
1:B:51:GLY:C	1:B:305:LEU:HG	2.42	0.43
2:N:145:TYR:OH	2:N:148:GLU:OE2	2.29	0.43
1:B:346:ALA:C	1:B:348:SER:H	2.26	0.43
1:C:64:ILE:HG23	1:C:204:LEU:HD11	1.99	0.43
1:C:345:ASN:OD1	1:C:346:ALA:N	2.51	0.43
4:D:12:VAL:HG11	4:D:82(C):LEU:HD12	2.00	0.43
4:D:148:GLU:CD	4:D:148:GLU:H	2.25	0.43
5:E:140:TYR:CD2	5:E:141:PRO:HA	2.53	0.43
3:M:2:ILE:O	3:M:97:THR:HG21	2.18	0.43
3:M:124:GLN:HG2	3:M:129:THR:O	2.18	0.43
2:N:89:THR:HA	2:N:108:THR:HA	2.00	0.43
1:A:49:ARG:HE	1:A:368:ASP:CG	2.26	0.43
1:A:329:GLY:O	1:A:331:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:NE	1:B:368:ASP:OD1	2.52	0.43
1:C:500:ASN:O	1:C:504:ALA:N	2.39	0.43
3:L:5:THR:HB	3:L:24:SER:OG	2.18	0.43
1:B:141:LEU:HD11	1:C:400:THR:HG21	2.00	0.43
1:B:368:ASP:HB3	1:B:371:ASN:OD1	2.19	0.43
4:H:195:ILE:HA	4:H:209:LYS:O	2.17	0.43
4:D:96:ARG:HG2	4:D:100(E):GLY:O	2.18	0.43
5:E:18:ARG:NH2	5:E:74:THR:HG21	2.33	0.43
2:K:70:SER:O	2:K:78:VAL:HG13	2.18	0.43
1:A:448:ASP:OD1	1:A:461:LYS:NZ	2.32	0.43
1:B:181:LEU:HA	1:B:181:LEU:HD23	1.59	0.43
3:L:12:SER:HB3	3:L:107:LYS:CG	2.43	0.43
5:I:140:TYR:CG	5:I:141:PRO:HA	2.54	0.43
1:B:338:ASP:OD1	1:B:338:ASP:N	2.45	0.43
4:H:52(A):TYR:CE2	4:H:53:ASP:HB3	2.54	0.43
4:H:97:ILE:HD12	4:H:100(D):TYR:CG	2.53	0.43
2:N:93:ALA:HB1	2:N:100(B):PHE:HB3	1.99	0.43
1:A:75:LYS:CB	1:A:214:ILE:HG21	2.46	0.43
1:A:378:GLU:OE1	1:A:378:GLU:N	2.52	0.43
1:A:407:ILE:HD12	1:C:146:SER:H	1.84	0.43
2:J:96:MET:HB2	2:J:99:ASN:OD1	2.18	0.43
5:G:105:GLU:HG3	5:G:173:TYR:HH	1.84	0.43
2:N:94:ARG:O	2:N:100(B):PHE:HA	2.18	0.43
1:A:414:VAL:O	1:A:439:CYS:HA	2.18	0.43
1:B:49:ARG:HG3	1:B:304:PRO:CB	2.48	0.43
1:B:329:GLY:C	1:B:331:ASN:H	2.26	0.43
2:K:154:TRP:C	2:K:156:SER:H	2.27	0.43
1:A:71:GLY:HA3	1:A:212:CYS:HB2	2.01	0.43
2:J:38:ARG:HG2	2:J:48:LEU:HD11	2.01	0.43
4:F:82:MET:HE2	4:F:82(C):LEU:HD21	2.00	0.43
4:D:185:PRO:O	4:D:188:SER:HB3	2.18	0.43
2:K:35:SER:HB3	2:K:95:ASP:HB3	2.00	0.43
2:N:64:LYS:CD	2:N:65:ASP:HA	2.49	0.43
2:N:168:ALA:HA	2:N:178:LEU:HB3	2.01	0.43
3:O:118:PHE:HA	3:O:119:PRO:HD2	1.90	0.43
1:A:252:LEU:O	1:A:282:ARG:NH2	2.36	0.43
1:B:161:GLU:HB2	1:B:162:GLY:H	1.58	0.43
4:F:82:MET:HB3	4:F:82(C):LEU:HD21	2.01	0.43
1:A:176:LYS:HE2	1:A:263:ASP:OD2	2.18	0.42
1:A:198:TYR:CD1	1:A:202:GLN:HG3	2.54	0.42
1:A:488:PHE:CZ	1:C:488:PHE:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:151:THR:OG1	2:N:199:ASN:HB3	2.19	0.42
3:O:4:MET:HE3	3:O:4:MET:HB3	1.81	0.42
1:A:315:LYS:HB2	1:A:341:TRP:CZ3	2.53	0.42
1:A:316:LEU:HD23	1:A:338:ASP:O	2.19	0.42
2:J:145:TYR:CZ	2:J:150:VAL:HG11	2.53	0.42
3:L:30:VAL:HG13	3:L:92:SER:OG	2.19	0.42
3:L:111:ALA:HB3	3:L:139:PHE:HA	2.01	0.42
3:L:163:VAL:HA	3:L:175:LEU:HA	2.01	0.42
4:F:117:LYS:HD3	4:F:175:LEU:HD21	2.00	0.42
5:G:93:ASN:HB3	5:G:94:LEU:H	1.47	0.42
5:G:108:ARG:HD2	5:G:171:SER:HB2	2.01	0.42
4:D:200:HIS:NE2	4:D:202:PRO:HG2	2.34	0.42
1:A:396:MET:HE3	1:A:488:PHE:HA	2.02	0.42
1:A:407:ILE:HD12	1:C:145:GLY:HA2	2.01	0.42
5:E:37:HIS:HB2	5:E:47:LEU:HD11	2.02	0.42
2:K:154:TRP:CZ3	2:K:196:CYS:HB3	2.54	0.42
1:A:146:SER:HB3	1:A:149:ALA:HB2	2.02	0.42
1:A:271:LYS:HB3	2:K:97:ILE:HD11	2.01	0.42
1:C:56:VAL:HG23	1:C:187:VAL:HG21	2.01	0.42
1:C:329:GLY:C	1:C:331:ASN:H	2.26	0.42
1:C:371:ASN:O	1:C:371:ASN:ND2	2.53	0.42
4:F:2:VAL:N	4:F:26:GLY:HA3	2.34	0.42
3:M:33:MET:C	3:M:34:HIS:CD2	2.97	0.42
1:A:218:GLU:OE2	1:C:75:LYS:HE3	2.18	0.42
1:C:161:GLU:HG2	4:H:27:PHE:CA	2.46	0.42
1:C:272:LYS:NZ	2:J:99:ASN:HA	2.35	0.42
1:A:379:VAL:HG22	1:A:391:TYR:CZ	2.54	0.42
1:B:61:LEU:N	1:B:295:GLU:O	2.42	0.42
1:B:240:ASN:HB3	1:B:243:VAL:O	2.20	0.42
1:B:374:THR:HG21	1:C:454:ASN:N	2.16	0.42
1:B:396:MET:HE3	1:B:488:PHE:HA	2.00	0.42
1:C:229:ARG:NH2	1:C:256:GLU:OE1	2.49	0.42
2:J:12:VAL:HG13	2:J:111:VAL:HG22	2.00	0.42
2:J:51:ILE:HD13	2:J:71:LYS:HB3	2.02	0.42
2:J:100(A):TYR:HD2	3:L:34:HIS:CE1	2.37	0.42
3:L:1:ASP:HA	3:L:95:PRO:HD2	2.02	0.42
1:A:66:GLU:OE2	1:A:66:GLU:N	2.52	0.42
1:B:178:VAL:CG1	1:B:188:LEU:HD12	2.50	0.42
4:F:195:ILE:HD11	4:F:208:ASP:HB3	2.01	0.42
5:G:150:VAL:HG22	5:G:192:TYR:CD2	2.54	0.42
2:K:64:LYS:CD	2:K:65:ASP:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:211:ARG:HB3	3:O:211:ARG:NH1	2.34	0.42
1:A:376:PRO:O	1:A:379:VAL:HG23	2.19	0.42
1:B:352:PHE:CE2	1:B:372:SER:HB3	2.54	0.42
1:B:370:MET:HE2	1:B:370:MET:HB3	1.94	0.42
1:C:208:ASN:HA	1:C:209:LYS:HA	1.63	0.42
1:C:352:PHE:HA	1:C:353:PRO:HD2	1.86	0.42
4:F:82(C):LEU:HD13	4:F:111:VAL:HG22	2.02	0.42
3:M:62:PHE:CD2	3:M:75:ILE:HG12	2.54	0.42
3:L:32:TYR:HB2	3:L:34:HIS:HE2	1.85	0.42
4:D:52(A):TYR:CD1	4:D:99:ASP:HA	2.55	0.42
5:E:108:ARG:NH1	5:E:111:ALA:HB2	2.34	0.42
1:C:264:MET:HA	1:C:265:PRO:HD3	1.87	0.42
1:C:323:THR:HG23	1:C:475:ILE:HG12	2.02	0.42
4:D:193:THR:HG23	4:D:210:LYS:HZ3	1.84	0.42
1:A:275:SER:O	1:C:95:LEU:HD21	2.19	0.41
1:B:176:LYS:HE2	1:B:263:ASP:OD2	2.20	0.41
4:F:185:PRO:O	4:F:188:SER:HB3	2.19	0.41
1:B:345:ASN:ND2	1:B:350:SER:OG	2.52	0.41
1:C:137:PHE:HE1	1:C:339:ARG:CZ	2.33	0.41
5:I:112:ALA:HB2	5:I:200:GLY:O	2.19	0.41
3:M:146:VAL:HG22	3:M:161:GLU:OE2	2.20	0.41
1:B:56:VAL:HG23	1:B:187:VAL:HG21	2.02	0.41
1:B:264:MET:HE1	1:B:274:MET:CE	2.51	0.41
4:F:36:TRP:O	4:F:48:VAL:HB	2.20	0.41
5:I:107:LYS:HG3	5:I:140:TYR:OH	2.19	0.41
5:I:151:ASP:HA	5:I:191:VAL:HG13	2.01	0.41
2:N:41:PRO:HD3	2:N:87:THR:O	2.20	0.41
2:N:66:ARG:O	2:N:82:VAL:HA	2.20	0.41
4:F:11:VAL:HG11	4:F:116:THR:OG1	2.20	0.41
4:H:163:VAL:HG22	4:H:182:VAL:HG22	2.03	0.41
3:M:146:VAL:HG11	3:M:175:LEU:HD21	2.03	0.41
1:C:193:LEU:HD23	1:C:193:LEU:HA	1.78	0.41
2:J:119:PRO:HB3	2:J:145:TYR:CB	2.39	0.41
4:D:143:LYS:HA	4:D:177:SER:HB2	2.02	0.41
3:M:11:LEU:HD12	3:M:12:SER:H	1.85	0.41
1:A:217:ILE:HD13	1:B:218:GLU:HG3	2.03	0.41
1:A:262:ASN:O	2:K:56:LYS:NZ	2.41	0.41
1:C:310:ASP:N	1:C:364:ARG:HH22	2.17	0.41
4:F:148:GLU:CD	4:F:148:GLU:H	2.27	0.41
5:I:124:GLN:HG2	5:I:129:THR:O	2.21	0.41
1:C:334:LEU:HD12	1:C:396:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:139:GLY:HA2	4:H:154:TRP:HH2	1.85	0.41
1:A:229:ARG:HH22	1:A:256:GLU:CD	2.28	0.41
1:A:352:PHE:CE2	1:A:372:SER:HB3	2.56	0.41
4:H:121:VAL:HG21	4:H:198:VAL:HG21	2.02	0.41
5:E:31:LYS:O	5:E:50:ASP:HA	2.21	0.41
2:N:146:PHE:HA	2:N:147:PRO:HA	1.86	0.41
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.94	0.41
1:C:137:PHE:CD1	1:C:137:PHE:N	2.88	0.41
1:C:289:MET:HE1	1:C:297:LEU:HD11	2.02	0.41
1:C:428:ASN:ND2	4:D:97:ILE:HD13	2.36	0.41
3:L:49:TYR:HE1	3:L:55:ALA:HA	1.86	0.41
5:I:118:PHE:HA	5:I:119:PRO:HD2	1.95	0.41
4:D:114:ALA:HB3	4:D:146:PHE:CE2	2.56	0.41
2:K:143:LYS:HG2	2:K:144:ASP:CG	2.46	0.41
3:M:6:GLN:OE1	3:M:99:GLY:HA3	2.20	0.41
2:N:61:PRO:HD2	3:O:95:PRO:CG	2.48	0.41
1:A:317:HIS:CG	1:A:408:THR:HG22	2.56	0.41
1:A:352:PHE:HA	1:A:353:PRO:HD2	1.88	0.41
1:C:280:ILE:HD11	1:C:361:GLN:HE21	1.86	0.41
4:F:28:SER:HB3	4:F:31:HIS:CD2	2.56	0.41
2:K:60:ASN:HA	2:K:61:PRO:HD3	1.88	0.41
3:O:30:VAL:HG13	3:O:92:SER:OG	2.21	0.41
1:A:496:ASN:O	1:A:500:ASN:N	2.43	0.40
1:B:491:SER:O	1:B:495:VAL:HG23	2.21	0.40
1:C:83:LEU:HD11	1:C:203:LEU:HD21	2.02	0.40
1:C:491:SER:O	1:C:495:VAL:HG23	2.21	0.40
2:J:30:SER:CB	2:J:73:THR:HG21	2.48	0.40
3:M:119:PRO:HB3	3:M:209:PHE:CE2	2.56	0.40
1:C:270:GLN:HG2	1:C:309:ILE:CD1	2.51	0.40
3:L:6:GLN:NE2	3:L:86:TYR:O	2.53	0.40
4:H:97:ILE:HD12	4:H:100(D):TYR:CD1	2.56	0.40
2:K:143:LYS:HZ3	3:M:129:THR:HG21	1.83	0.40
1:C:163:GLU:HG3	1:C:181:LEU:HD22	2.03	0.40
1:C:335:THR:HB	1:C:396:MET:HG2	2.03	0.40
2:J:125:ALA:HA	2:J:126:PRO:HD3	1.76	0.40
5:G:108:ARG:HH11	5:G:108:ARG:HG3	1.86	0.40
2:K:118:GLY:HA2	2:K:119:PRO:HD3	1.93	0.40
2:N:22:CYS:O	2:N:77:GLN:HA	2.20	0.40
3:O:54:LEU:HD11	3:O:60:SER:HA	2.03	0.40
3:O:122:ASP:O	3:O:126:LYS:HG3	2.22	0.40
1:A:262:ASN:ND2	2:K:53:TRP:HH2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:SER:OG	1:B:471:GLY:HA3	2.21	0.40
1:B:217:ILE:HG13	1:B:220:VAL:HG22	2.02	0.40
1:B:321:LEU:HD11	1:B:473:PRO:HB3	2.03	0.40
1:C:178:VAL:CG1	1:C:188:LEU:HD12	2.51	0.40
2:J:143:LYS:HZ3	3:L:129:THR:HG21	1.81	0.40
3:L:13:ALA:H	3:L:106:ILE:HA	1.87	0.40
2:K:22:CYS:HB2	2:K:36:TRP:CZ2	2.57	0.40
2:K:66:ARG:NH2	2:K:86:ASP:OD2	2.44	0.40
3:M:63:SER:OG	3:M:74:THR:HB	2.21	0.40
3:M:142:ARG:NH2	3:M:163:VAL:HG11	2.37	0.40
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.87	0.40
1:B:324:THR:HG21	1:B:437:ASN:O	2.21	0.40
4:D:27:PHE:CE2	4:D:29:PHE:HA	2.57	0.40
5:E:78:LEU:CD2	5:E:106:ILE:HG13	2.52	0.40
3:M:7:SER:HA	3:M:8:PRO:C	2.47	0.40
2:N:64:LYS:HD2	2:N:64:LYS:HA	1.82	0.40

All (1) 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)
3:L:145:LYS:NZ	3:O:17:ASP:OD1[2_645]	2.18	0.02

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	445/498 (89%)	410 (92%)	29 (6%)	6 (1%)	9	41
1	B	445/498 (89%)	410 (92%)	29 (6%)	6 (1%)	9	41
1	C	445/498 (89%)	411 (92%)	28 (6%)	6 (1%)	9	41
2	J	209/225 (93%)	192 (92%)	16 (8%)	1 (0%)	24	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	209/225 (93%)	193 (92%)	14 (7%)	2 (1%)	12	48
2	N	209/225 (93%)	196 (94%)	13 (6%)	0	100	100
3	L	209/213 (98%)	195 (93%)	13 (6%)	1 (0%)	24	64
3	M	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
3	O	209/213 (98%)	200 (96%)	9 (4%)	0	100	100
4	D	212/227 (93%)	208 (98%)	4 (2%)	0	100	100
4	F	212/227 (93%)	208 (98%)	4 (2%)	0	100	100
4	H	212/227 (93%)	205 (97%)	7 (3%)	0	100	100
5	E	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
5	G	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
5	I	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
All	All	3858/4134 (93%)	3633 (94%)	203 (5%)	22 (1%)	21	59

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	161	GLU
1	B	50	THR
1	B	161	GLU
1	C	50	THR
1	C	161	GLU
1	A	214	ILE
1	B	214	ILE
1	C	71	GLY
2	J	156	SER
2	K	156	SER
1	A	210	GLN
1	A	437	ASN
1	B	210	GLN
1	C	216	ASN
1	C	437	ASN
1	B	437	ASN
1	C	65	LYS
3	L	78	LEU
1	A	490	ALA
1	B	490	ALA
2	K	119	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/448 (92%)	391 (95%)	19 (5%)	24	45
1	B	410/448 (92%)	375 (92%)	35 (8%)	10	29
1	C	410/448 (92%)	375 (92%)	35 (8%)	10	29
2	J	187/197 (95%)	182 (97%)	5 (3%)	39	60
2	K	187/197 (95%)	183 (98%)	4 (2%)	47	65
2	N	187/197 (95%)	180 (96%)	7 (4%)	30	51
3	L	183/185 (99%)	177 (97%)	6 (3%)	33	55
3	M	183/185 (99%)	176 (96%)	7 (4%)	29	50
3	O	183/185 (99%)	176 (96%)	7 (4%)	29	50
4	D	182/192 (95%)	177 (97%)	5 (3%)	39	60
4	F	182/192 (95%)	177 (97%)	5 (3%)	39	60
4	H	181/192 (94%)	175 (97%)	6 (3%)	33	55
5	E	189/191 (99%)	187 (99%)	2 (1%)	65	75
5	G	189/191 (99%)	187 (99%)	2 (1%)	65	75
5	I	189/191 (99%)	187 (99%)	2 (1%)	65	75
All	All	3452/3639 (95%)	3305 (96%)	147 (4%)	26	47

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	67	ASN
1	A	77	LYS
1	A	95	LEU
1	A	155	CYS
1	A	167	ILE
1	A	169	SER
1	A	202	GLN
1	A	203	LEU
1	A	216	ASN

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Mol	Chain	Res	Type
1	A	217	ILE
1	A	220	VAL
1	A	260	LEU
1	A	292	ILE
1	A	297	LEU
1	A	380	ASN
1	A	449	THR
1	A	459	VAL
1	A	486	ASP
1	B	60	GLU
1	B	67	ASN
1	B	77	LYS
1	B	95	LEU
1	B	96	LEU
1	B	137	PHE
1	B	138	LEU
1	B	155	CYS
1	B	158	LEU
1	B	160	LEU
1	B	161	GLU
1	B	167	ILE
1	B	169	SER
1	B	180	SER
1	B	193	LEU
1	B	202	GLN
1	B	203	LEU
1	B	216	ASN
1	B	217	ILE
1	B	220	VAL
1	B	232	GLU
1	B	234	THR
1	B	260	LEU
1	B	279	GLN
1	B	289	MET
1	B	292	ILE
1	B	297	LEU
1	B	357	THR
1	B	364	ARG
1	B	380	ASN
1	B	386	ILE
1	B	449	THR
1	B	459	VAL

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Mol	Chain	Res	Type
1	B	467	LEU
1	B	486	ASP
1	C	60	GLU
1	C	68	LYS
1	C	70	ASN
1	C	80	LYS
1	C	95	LEU
1	C	96	LEU
1	C	137	PHE
1	C	138	LEU
1	C	155	CYS
1	C	158	LEU
1	C	160	LEU
1	C	161	GLU
1	C	167	ILE
1	C	169	SER
1	C	193	LEU
1	C	203	LEU
1	C	204	LEU
1	C	214	ILE
1	C	232	GLU
1	C	234	THR
1	C	260	LEU
1	C	279	GLN
1	C	289	MET
1	C	292	ILE
1	C	297	LEU
1	C	357	THR
1	C	364	ARG
1	C	380	ASN
1	C	386	ILE
1	C	405	SER
1	C	436	SER
1	C	440	ASP
1	C	449	THR
1	C	459	VAL
1	C	486	ASP
2	J	4	LEU
2	J	29	LEU
2	J	48	LEU
2	J	67	LEU
2	J	197	ASN

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Mol	Chain	Res	Type
3	L	30	VAL
3	L	136	LEU
3	L	146	VAL
3	L	163	VAL
3	L	164	THR
3	L	191	VAL
4	F	12	VAL
4	F	120	SER
4	F	138	LEU
4	F	148	GLU
4	F	209	LYS
5	G	89	GLN
5	G	191	VAL
4	H	12	VAL
4	H	116	THR
4	H	120	SER
4	H	138	LEU
4	H	148	GLU
4	H	209	LYS
5	I	89	GLN
5	I	191	VAL
4	D	12	VAL
4	D	120	SER
4	D	138	LEU
4	D	148	GLU
4	D	209	LYS
5	E	89	GLN
5	E	191	VAL
2	K	4	LEU
2	K	29	LEU
2	K	48	LEU
2	K	67	LEU
3	M	30	VAL
3	M	107	LYS
3	M	136	LEU
3	M	146	VAL
3	M	163	VAL
3	M	164	THR
3	M	191	VAL
2	N	1	GLN
2	N	29	LEU
2	N	48	LEU

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Mol	Chain	Res	Type
2	N	67	LEU
2	N	97	ILE
2	N	150	VAL
2	N	169	VAL
3	O	10	THR
3	O	60	SER
3	O	136	LEU
3	O	146	VAL
3	O	163	VAL
3	O	164	THR
3	O	191	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	67	ASN
1	A	197	ASN
1	A	216	ASN
1	A	225	GLN
1	A	227	ASN
1	A	262	ASN
1	A	270	GLN
1	A	276	ASN
1	A	354	GLN
1	A	454	ASN
1	A	476	ASN
1	B	26	GLN
1	B	34	GLN
1	B	67	ASN
1	B	202	GLN
1	B	216	ASN
1	B	270	GLN
1	B	276	ASN
1	B	363	ASN
1	C	26	GLN
1	C	70	ASN
1	C	81	GLN
1	C	175	ASN
1	C	240	ASN
1	C	262	ASN
1	C	268	ASN

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Mol	Chain	Res	Type
1	C	270	GLN
1	C	276	ASN
1	C	354	GLN
1	C	363	ASN
1	C	428	ASN
1	C	454	ASN
2	J	39	GLN
2	J	58	HIS
3	L	38	GLN
3	L	137	ASN
3	L	138	ASN
4	F	31	HIS
4	F	39	GLN
5	G	38	GLN
5	G	210	ASN
4	H	39	GLN
5	I	3	GLN
5	I	38	GLN
5	I	137	ASN
4	D	31	HIS
4	D	39	GLN
4	D	81	GLN
4	D	82(A)	ASN
4	D	155	ASN
5	E	38	GLN
5	E	79	GLN
5	E	210	ASN
2	K	58	HIS
3	M	124	GLN
3	M	137	ASN
2	N	58	HIS
3	O	138	ASN
3	O	160	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	449/498 (90%)	-0.09	4 (0%) 81 69	152, 187, 250, 286	0
1	B	449/498 (90%)	-0.19	2 (0%) 88 78	156, 197, 266, 334	0
1	C	449/498 (90%)	-0.23	3 (0%) 84 73	140, 186, 235, 255	0
2	J	213/225 (94%)	-0.34	3 (1%) 73 61	148, 170, 197, 213	0
2	K	213/225 (94%)	-0.34	0 100 100	164, 209, 288, 297	0
2	N	213/225 (94%)	-0.33	4 (1%) 66 55	191, 238, 277, 289	0
3	L	211/213 (99%)	-0.17	1 (0%) 87 77	148, 195, 226, 253	0
3	M	211/213 (99%)	-0.19	0 100 100	177, 245, 273, 284	0
3	O	211/213 (99%)	-0.30	0 100 100	204, 239, 271, 298	0
4	D	216/227 (95%)	-0.19	2 (0%) 81 69	193, 269, 359, 370	0
4	F	216/227 (95%)	-0.14	3 (1%) 73 61	192, 234, 280, 287	0
4	H	216/227 (95%)	-0.09	2 (0%) 81 69	151, 183, 202, 211	0
5	E	213/215 (99%)	-0.05	4 (1%) 66 55	221, 305, 367, 382	0
5	G	213/215 (99%)	-0.11	6 (2%) 55 47	211, 250, 279, 297	0
5	I	213/215 (99%)	-0.14	4 (1%) 66 55	155, 191, 214, 231	0
All	All	3906/4134 (94%)	-0.19	38 (0%) 79 67	140, 208, 316, 382	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	ASP	4.1
1	A	488	PHE	3.8
5	I	136	LEU	3.7
5	G	73	LEU	3.4
2	J	137	ALA	3.3
2	J	18	LEU	3.2
5	G	21	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	N	33	GLY	3.0
1	A	137	PHE	3.0
5	I	135	LEU	2.8
2	N	34	MET	2.8
2	N	32	ALA	2.7
5	E	131	SER	2.5
4	H	100(F)	MET	2.5
5	E	100	GLY	2.5
5	G	35	TRP	2.4
4	F	172	SER	2.4
1	C	421	LYS	2.3
4	F	173	SER	2.3
5	E	212	GLY	2.2
2	N	127	SER	2.2
3	L	13	ALA	2.1
4	H	134	GLY	2.1
5	E	178	THR	2.1
4	D	85	GLU	2.1
4	D	127	SER	2.1
5	I	208	SER	2.1
5	I	165	GLU	2.1
1	C	218	GLU	2.1
4	F	120	SER	2.1
2	J	12	VAL	2.1
5	G	106	ILE	2.0
5	G	109	THR	2.0
1	B	260	LEU	2.0
1	B	488	PHE	2.0
1	C	281	VAL	2.0
1	A	487	GLU	2.0
5	G	180	THR	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.