Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 04:32 AM EDT

PDB ID	:	4ZYP
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 (i) 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 (1)) were used in the production of this report:

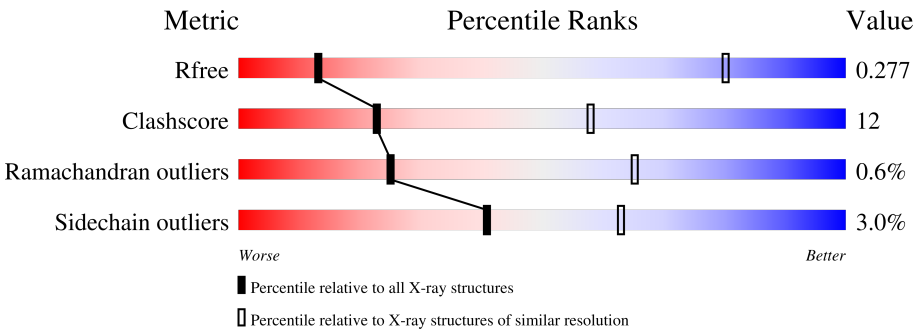
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	498	61% 27% • 10%
1	B	498	61% 26% • 10%
1	C	498	59% 27% • 10%
2	J	225	64% 29% • 5%
2	K	225	62% 31% • 5%
2	N	225	70% 24% 5%
3	L	213	73% 25% •

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Mol	Chain	Length	Quality of chain
3	M	213	72% 25%
3	O	213	86% 12%
4	D	227	77% 17% 5%
4	F	227	74% 21% 5%
4	H	227	74% 21% 5%
5	E	215	80% 19%
5	G	215	84% 14%
5	I	215	78% 20%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	449	3482	2202	573	684	23	0	0	0
1	B	449	3482	2202	573	684	23	0	0	0
1	C	449	3482	2202	573	684	23	0	0	0

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
			Total	C	N	O	S			
2	J	213	1626	1039	266	314	7	0	0	0
2	K	213	1626	1039	266	314	7	0	0	0
2	N	213	1626	1039	266	314	7	0	0	0

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

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

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

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

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

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

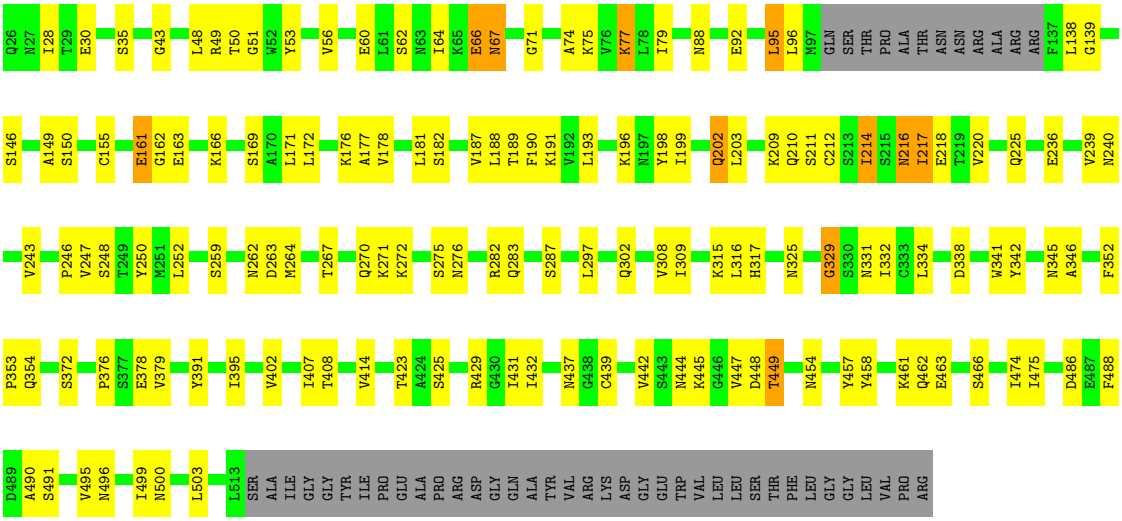
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	G	213	1642	1025	277	334	6	0	0	0
5	I	213	1642	1025	277	334	6	0	0	0
5	E	213	1642	1025	277	334	6	0	0	0

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. 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. 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.

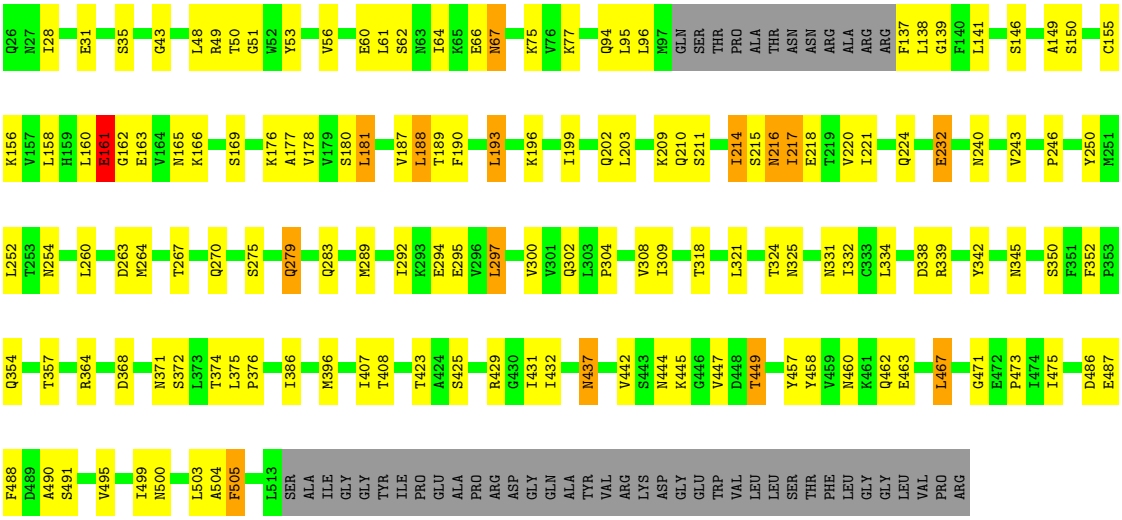
• Molecule 1: Fusion glycoprotein F0,Fibritin

Chain A:



• Molecule 1: Fusion glycoprotein F0,Fibritin

Chain B:



• Molecule 1: Fusion glycoprotein F0,Fibritin

Chain C: 59% 27% • 10%

Q26 N27 I28 S35 G43 L48 R49 T50 G51 V56 E60 L61 S62 N63 I64 K65 E66 N67 K68 C69 N70 G71 T72 D73 A74 K75 V76 Q81 E82 L83 L93 Q94 L95 L96 M97 GLN SER THR PRO ALA THR ASN ASN ARG ALA ARG ARG F137 L138 G139 G145 S146

A149 C155 K156 V157 L158 H159 L160 E161 G162 E163 V164 N165 K166 S169 A177 V178 L181 S182 N183 G184 V185 S186 V187 L188 T189 L193 D194 L195 K196 L203 L204 P205 I206 L207 N208 K209 I214 S215 N216 I217 E218 K226 R229 E232 R235 V239 N240

V243 P246 Y250 M251 L252 E256 L260 I261 N262 D263 M264 P265 I266 T267 Q270 K271 K272 Q279 I280 Q283 M289 I292 K293 E294 L297 V300 V301 V308 I309 D310 T318 C322 T323 T324 I332 C333 L334 T335 R339 N345 A346

F352 P353 Q354 T357 Q361 S362 N363 R364 D368 N371 S372 L373 T374 L375 P376 V379 I386 M396 T400 S405 Y406 I407 T408 T423 A424 S425 N428 R429 G430 I431 I432 S436 N437 D440 Y441 V442 K445 G446 V447 D448 T449 N454 Y457 Y458

V459 N460 K461 Q462 E463 I474 I475 D486 E487 F488 S491 V495 K498 I499 N500 L503 A504 F505 L513 SER ALA ILE GLY GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY GLY LEU

VAL PRO ARG

• Molecule 2: Motavizumab antibody Fab heavy chain

Chain J: 64% 29% • 5%

Q1 L4 R5 E6 V12 K13 P14 T15 Q16 C22 T23 F24 L29 S30 G33 M34 S35 W36 I37 R38 Q39 P40 K43 A44 L45 L48 I51 W52 K56 K64 D65 R66 L67 K71 D72 T73 P84 T89 A93 R94 D95 M96 I97 F98 N99

F100 Y100A T108 V111 K117 G118 P119 P123 L124 A125 P126 S127 SER LYS SER THR SER GLY GLY T135 A136 A137 L138 G139 C140 L141 V142 K143 D144 Y145 V150 S156 L159 V163 A168 Q171 L178 V182 T183 S188 Q192 I195 C196 N197 V198

N199 S203 K206 V207 D208 K209 P213 LYS SER CYS ASP LYS

• Molecule 2: Motavizumab antibody Fab heavy chain

Chain K: 62% 31% • 5%

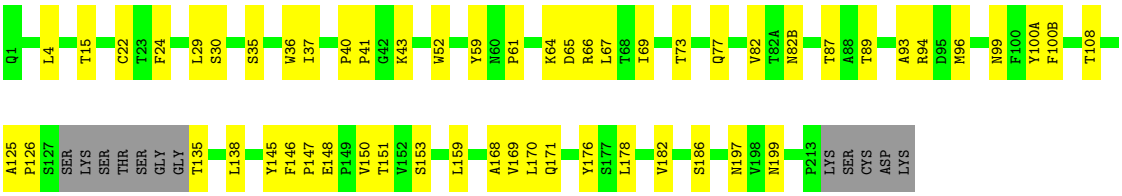
Q1 V2 T3 L4 R5 E6 V12 L20 T21 C22 T23 F24 S25 L29 S30 S35 W36 I37 R38 Q39 L45 L48 I51 W52 W53 K56 N60 P61 K64 D65 R66 L67 S70 K71 D72 T73 V78 V79 P84 A85 D86 T89 D95 M96

I97 F98 N99 F100 Y100A T108 V111 G118 P119 F122 P123 L124 A125 P126 S127 SER LYS SER THR SER GLY GLY T135 A136 A137 L138 G139 C140 L141 V142 K143 D144 Y145 W154 N155 S156 L159 V163 Q171 L175 S179 V182 T183 I195 C196 H200 K201

P202 S203 K209 K210 V211 E212 P213 LYS SER CYS ASP LYS

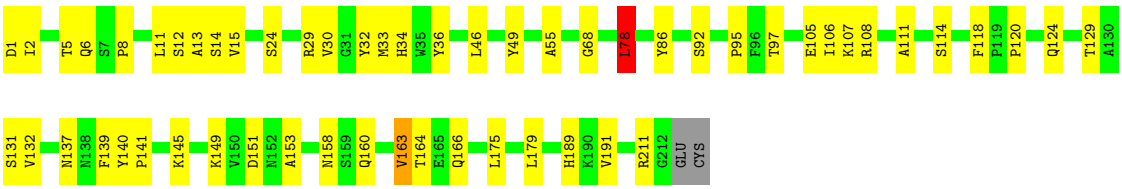
• Molecule 2: Motavizumab antibody Fab heavy chain

Chain N: 70% 24% 5%



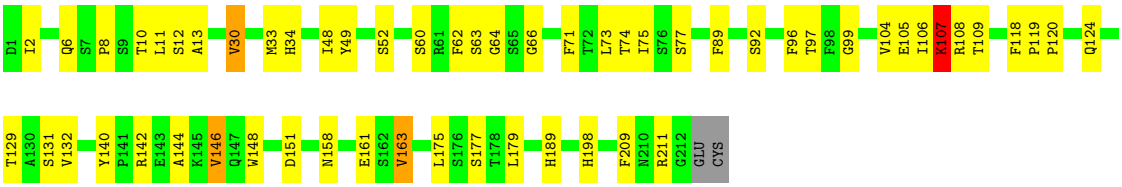
• Molecule 3: Motavizumab antibody light chain

Chain L: 73% 25%



• Molecule 3: Motavizumab antibody light chain

Chain M: 72% 25%

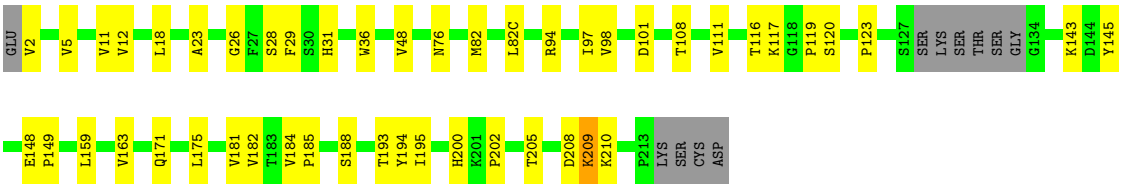


• Molecule 3: Motavizumab antibody light chain

Chain O: 86% 12%

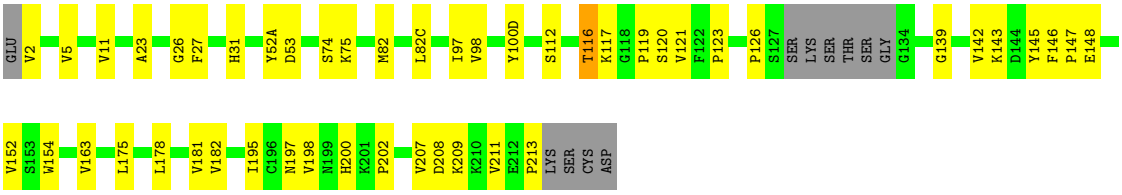
• Molecule 4: AM14 antibody Fab heavy chain

Chain F: 74% 21% 5%



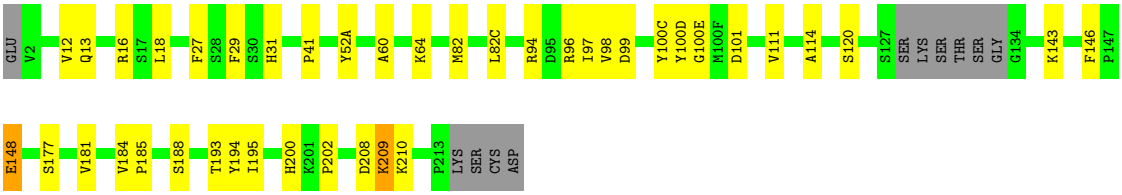
• Molecule 4: AM14 antibody Fab heavy chain

Chain H: 74% 21% 5%



- Molecule 4: AM14 antibody Fab heavy chain

Chain D:

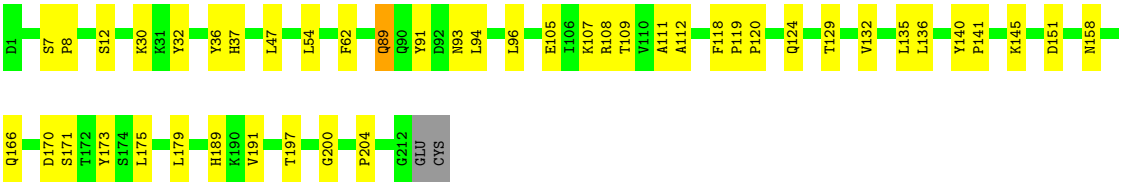


- Molecule 5: AM14 antibody light chain

Chain G:

- Molecule 5: AM14 antibody light chain

Chain I:



- Molecule 5: AM14 antibody light chain

Chain E:

4 Data and refinement statistics (i)

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 49.59 – 5.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.39-5.50) 97.2 (49.59-5.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 5.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.277 0.214 , 0.277	Depositor DCC
R_{free} test set	857 reflections (4.92%)	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)	0.26 , 185.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.35	0/3532	0.67	1/4784 (0.0%)
1	B	0.34	0/3532	0.68	2/4784 (0.0%)
1	C	0.35	0/3532	0.71	1/4784 (0.0%)
2	J	0.40	0/1669	0.83	2/2283 (0.1%)
2	K	0.33	0/1669	0.73	1/2283 (0.0%)
2	N	0.29	0/1669	0.51	0/2283
3	L	0.34	0/1648	0.69	1/2235 (0.0%)
3	M	0.33	0/1648	0.71	1/2235 (0.0%)
3	O	0.29	0/1648	0.52	0/2235
4	D	0.28	0/1677	0.51	0/2286
4	F	0.28	0/1677	0.49	0/2286
4	H	0.31	0/1676	0.64	0/2285
5	E	0.33	0/1677	0.64	0/2277
5	G	0.26	0/1677	0.50	0/2277
5	I	0.30	0/1677	0.57	0/2277
All	All	0.33	0/30608	0.65	9/41594 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	107	LYS	N-CA-C	6.15	127.61	111.00
1	B	181	LEU	CA-CB-CG	-5.93	101.65	115.30
2	J	178	LEU	CA-CB-CG	5.85	128.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	329	GLY	N-CA-C	-5.50	99.34	113.10
1	B	188	LEU	CA-CB-CG	5.41	127.73	115.30
1	C	181	LEU	CA-CB-CG	-5.35	103.00	115.30
2	J	141	LEU	CA-CB-CG	5.25	127.38	115.30
2	K	141	LEU	CA-CB-CG	5.24	127.35	115.30
3	L	164	THR	N-CA-C	5.20	125.04	111.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3482	0	3526	107	0
1	B	3482	0	3526	96	0
1	C	3482	0	3526	114	0
2	J	1626	0	1610	55	0
2	K	1626	0	1610	62	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	19	1
4	D	1636	0	1579	28	0
4	F	1636	0	1579	30	0
4	H	1635	0	1576	34	0
5	E	1642	0	1597	35	0
5	G	1642	0	1597	20	0
5	I	1642	0	1597	31	0
All	All	29990	0	29625	686	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 (686) 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
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
3:M:13:ALA:H	3:M:107:LYS:HZ3	1.25	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
3:M:13:ALA:H	3:M:107:LYS:NZ	1.93	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
1:B:64:ILE:HD11	1:B:199:ILE:HG21	1.78	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:C:49:ARG:O	1:C:49:ARG:HG2	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ILE:HG22	1:C:475:ILE:HD11	1.83	0.60
3:L:105:GLU:CD	3:L:106:ILE:H	2.03	0.60
1:A:182:SER:O	4:F:97:ILE:HA	2.00	0.60
2:N:135:THR:N	2:N:186:SER:HG	1.99	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
4:F:31:HIS:HB3	4:F:98:VAL:HG13	1.83	0.60
4:D:209:LYS:NZ	5:E:123:GLU:OE1	2.24	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
1:A:445:LYS:HZ3	1:A:463:GLU:HA	1.67	0.59
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
3:M:13:ALA:N	3:M:107:LYS:HZ3	1.96	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
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
3:M:11:LEU:HB3	3:M:104:VAL:HG22	1.86	0.58
1:C:445:LYS:HZ3	1:C:463:GLU:HA	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:I:108:ARG:O	5:I:109:THR:OG1	2.20	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:L:105:GLU:CD	3:L:166:GLN:HE22	2.10	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:143:LYS:HZ1	3:L:129:THR:HG21	1.74	0.52
4:F:29:PHE:CD2	4:F:76:ASN:HA	2.45	0.52
3:M:12:SER:HA	3:M:107:LYS:HZ3	1.75	0.52
2:J:35:SER:HB3	2:J:95:ASP:HB3	1.92	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
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
2:J:143:LYS:HZ3	3:L:129:THR:HG21	1.75	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
4:D:13:GLN:HB2	4:D:16:ARG:HD2	1.91	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
5:I:12:SER:OG	5:I:105:GLU:OE1	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:166:GLN:HE21	5:E:171:SER:C	2.15	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
1:B:177:ALA:O	1:B:189:THR:OG1	2.26	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
4:F:82:MET:HE2	4:F:82(C):LEU:HD21	1.95	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
1:C:279:GLN:CD	1:C:279:GLN:H	2.16	0.48
1:B:279:GLN:CD	1:B:279:GLN:H	2.16	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:49:ARG:HE	1:B:368:ASP:CG	2.16	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
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
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
3:M:105:GLU:C	3:M:107:LYS:HZ1	2.16	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
1:C:49:ARG:HE	1:C:368:ASP:CG	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:O:33:MET:C	3:O:34:HIS:HD2	2.18	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
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
1:A:329:GLY:C	1:A:331:ASN:H	2.18	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:448:ASP:OD1	1:A:461:LYS:NZ	2.32	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
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
3:O:4:MET:HB3	3:O:4:MET:HE3	1.59	0.45
1:A:272:LYS:HZ3	2:K:99:ASN:HA	1.81	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
1:C:195:LEU:CD2	1:C:226:LYS:HB3	2.46	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:K:4:LEU:HD23	2:K:24:PHE:CB	2.37	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
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
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
1:B:264:MET:HE2	1:B:264:MET:HB2	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:145:TYR:OH	2:N:148:GLU:OE2	2.29	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
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:329:GLY:O	1:A:331:ASN:N	2.51	0.43
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:75:LYS:NZ	1:B:215:SER:O	2.38	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:F:193:THR:HG23	4:F:210:LYS:HZ2	1.83	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
3:M:33:MET:C	3:M:34:HIS:HD2	2.21	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
1:C:272:LYS:HZ2	2:J:99:ASN:HA	1.83	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
3:L:33:MET:C	3:L:34:HIS:HD2	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:262:ASN:O	2:K:56:LYS:NZ	2.41	0.42
1:A:488:PHE:CZ	1:C:488:PHE:HB2	2.54	0.42
2:N:151:THR:OG1	2:N:199:ASN:HB3	2.19	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
1:C:261:ILE:HA	1:C:264:MET:HE2	2.02	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
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
5:E:105:GLU:HG2	5:E:166:GLN:CD	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:163:VAL:HG22	4:H:182:VAL:HG22	2.03	0.41
4:D:82:MET:HE2	4:D:82(C):LEU:HD21	2.03	0.41
3:M:146:VAL:HG11	3:M:175:LEU:HD21	2.03	0.41
1:A:264:MET:HB2	1:A:264:MET:HE2	1.74	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
2:N:36:TRP:C	2:N:37:ILE:HG13	2.41	0.41
1:A:217:ILE:HD13	1:B:218:GLU:HG3	2.03	0.41
1:C:310:ASP:N	1:C:364:ARG:HH22	2.17	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
2:J:36:TRP:C	2:J:37:ILE:HG13	2.41	0.41
4:H:139:GLY:HA2	4:H:154:TRP:HH2	1.85	0.41
3:M:107:LYS:HD3	3:M:140:TYR:HH	1.85	0.41
1:A:329:GLY:C	1:A:331:ASN:N	2.74	0.41
1:A:352:PHE:CE2	1:A:372:SER:HB3	2.56	0.41
1:B:445:LYS:HZ3	1:B:463:GLU:HA	1.86	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: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
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:264:MET:HE2	1:C:264:MET:HB2	1.81	0.40
1:C:491:SER:O	1:C:495:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:TRP:C	2:K:37:ILE:HG13	2.41	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
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
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
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%)	12	47
1	B	445/498 (89%)	410 (92%)	29 (6%)	6 (1%)	12	47
1	C	445/498 (89%)	411 (92%)	28 (6%)	6 (1%)	12	47
2	J	209/225 (93%)	192 (92%)	16 (8%)	1 (0%)	29	69
2	K	209/225 (93%)	193 (92%)	14 (7%)	2 (1%)	15	53
2	N	209/225 (93%)	196 (94%)	13 (6%)	0	100	100
3	L	209/213 (98%)	195 (93%)	13 (6%)	1 (0%)	29	69
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%)	25	65

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/448 (92%)	396 (97%)	14 (3%)	37	60
1	B	410/448 (92%)	382 (93%)	28 (7%)	16	42
1	C	410/448 (92%)	381 (93%)	29 (7%)	14	41
2	J	187/197 (95%)	184 (98%)	3 (2%)	62	79
2	K	187/197 (95%)	184 (98%)	3 (2%)	62	79
2	N	187/197 (95%)	183 (98%)	4 (2%)	53	72
3	L	183/185 (99%)	182 (100%)	1 (0%)	88	93
3	M	183/185 (99%)	179 (98%)	4 (2%)	52	71
3	O	183/185 (99%)	179 (98%)	4 (2%)	52	71
4	D	182/192 (95%)	179 (98%)	3 (2%)	62	79
4	F	182/192 (95%)	179 (98%)	3 (2%)	62	79
4	H	181/192 (94%)	178 (98%)	3 (2%)	60	78
5	E	189/191 (99%)	187 (99%)	2 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	189/191 (99%)	187 (99%)	2 (1%)	73	84
5	I	189/191 (99%)	188 (100%)	1 (0%)	88	93
All	All	3452/3639 (95%)	3348 (97%)	104 (3%)	41	63

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	66	GLU
1	A	67	ASN
1	A	77	LYS
1	A	95	LEU
1	A	155	CYS
1	A	169	SER
1	A	202	GLN
1	A	203	LEU
1	A	216	ASN
1	A	217	ILE
1	A	297	LEU
1	A	449	THR
1	A	486	ASP
1	B	60	GLU
1	B	67	ASN
1	B	77	LYS
1	B	95	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	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	232	GLU
1	B	279	GLN
1	B	289	MET

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Mol	Chain	Res	Type
1	B	297	LEU
1	B	357	THR
1	B	364	ARG
1	B	386	ILE
1	B	449	THR
1	B	467	LEU
1	B	486	ASP
1	B	505	PHE
1	C	60	GLU
1	C	65	LYS
1	C	68	LYS
1	C	70	ASN
1	C	95	LEU
1	C	137	PHE
1	C	155	CYS
1	C	158	LEU
1	C	160	LEU
1	C	161	GLU
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	260	LEU
1	C	279	GLN
1	C	289	MET
1	C	297	LEU
1	C	357	THR
1	C	364	ARG
1	C	386	ILE
1	C	405	SER
1	C	436	SER
1	C	440	ASP
1	C	449	THR
1	C	486	ASP
1	C	505	PHE
2	J	29	LEU
2	J	67	LEU
2	J	197	ASN
3	L	163	VAL
4	F	120	SER

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Mol	Chain	Res	Type
4	F	148	GLU
4	F	209	LYS
5	G	89	GLN
5	G	191	VAL
4	H	116	THR
4	H	120	SER
4	H	148	GLU
5	I	89	GLN
4	D	120	SER
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	67	LEU
3	M	30	VAL
3	M	107	LYS
3	M	146	VAL
3	M	163	VAL
2	N	29	LEU
2	N	67	LEU
2	N	150	VAL
2	N	169	VAL
3	O	10	THR
3	O	60	SER
3	O	146	VAL
3	O	163	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	67	ASN
1	A	165	ASN
1	A	197	ASN
1	A	202	GLN
1	A	216	ASN
1	A	227	ASN
1	A	262	ASN
1	A	270	GLN
1	A	276	ASN

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Mol	Chain	Res	Type
1	A	354	GLN
1	A	454	ASN
1	B	26	GLN
1	B	67	ASN
1	B	202	GLN
1	B	216	ASN
1	B	262	ASN
1	B	270	GLN
1	B	276	ASN
1	B	354	GLN
1	B	363	ASN
1	C	26	GLN
1	C	70	ASN
1	C	81	GLN
1	C	262	ASN
1	C	268	ASN
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	197	ASN
3	L	137	ASN
3	L	138	ASN
4	F	31	HIS
5	G	210	ASN
5	I	137	ASN
4	D	31	HIS
4	D	81	GLN
5	E	210	ASN
2	K	197	ASN
3	M	124	GLN
3	O	160	GLN

5.3.3 RNA (i)

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.