Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:42 PM GMT

PDB ID	:	4TNV
Title	:	C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab in a non-conducting conformation
Authors	:	Althoff, T.; Hibbs, R.E.; Banerjee, S.; Gouaux, E.
Deposited on	:	2014-06-05
Resolution	:	3.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

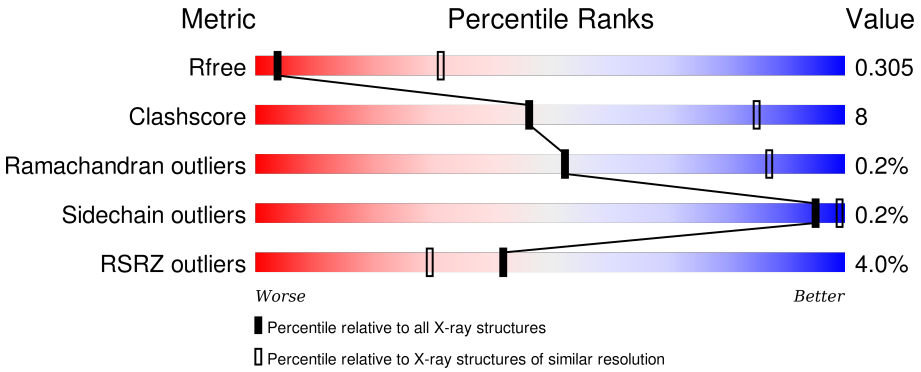
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	347	% 77% 20% ·
1	B	347	4% 76% 22% ·
1	C	347	% 77% 20% ·
1	D	347	3% 74% 23% ·
1	E	347	5% 76% 21% ·

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Mol	Chain	Length	Quality of chain
1	P	347	2% 75% 22%
1	Q	347	2% 76% 22%
1	R	347	% 76% 21%
1	S	347	2% 76% 21%
1	T	347	% 77% 20%
2	F	224	3% 81% 18%
2	G	224	5% 87% 13%
2	H	224	77% 22%
2	I	224	3% 87% 12%
2	J	224	13% 83% 17%
2	U	224	11% 83% 16%
2	V	224	5% 82% 17%
2	W	224	3% 75% 25%
2	X	224	% 86% 14%
2	Y	224	15% 83% 15%
3	K	215	3% 83% 15%
3	L	215	75% 23%
3	M	215	10% 85% 13%
3	N	215	2% 81% 17%
3	O	215	% 83% 15%
3	Z	215	2% 89% 11%
3	f	215	2% 99%
3	g	215	17% 98%
3	h	215	6% 98%
3	i	215	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 60408 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 Avermectin-sensitive glutamate-gated chloride channel GluCl alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	B	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	C	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	D	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	E	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	P	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	Q	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	R	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	S	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	T	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	ALA	-	linker	UNP G5EBR3
A	304	GLY	-	linker	UNP G5EBR3
A	305	THR	-	linker	UNP G5EBR3
A	340	HIS	-	expression tag	UNP G5EBR3
A	341	HIS	-	expression tag	UNP G5EBR3
A	342	HIS	-	expression tag	UNP G5EBR3
A	343	HIS	-	expression tag	UNP G5EBR3
A	344	HIS	-	expression tag	UNP G5EBR3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	345	HIS	-	expression tag	UNP G5EBR3
A	346	HIS	-	expression tag	UNP G5EBR3
A	347	HIS	-	expression tag	UNP G5EBR3
B	303	ALA	-	linker	UNP G5EBR3
B	304	GLY	-	linker	UNP G5EBR3
B	305	THR	-	linker	UNP G5EBR3
B	340	HIS	-	expression tag	UNP G5EBR3
B	341	HIS	-	expression tag	UNP G5EBR3
B	342	HIS	-	expression tag	UNP G5EBR3
B	343	HIS	-	expression tag	UNP G5EBR3
B	344	HIS	-	expression tag	UNP G5EBR3
B	345	HIS	-	expression tag	UNP G5EBR3
B	346	HIS	-	expression tag	UNP G5EBR3
B	347	HIS	-	expression tag	UNP G5EBR3
C	303	ALA	-	linker	UNP G5EBR3
C	304	GLY	-	linker	UNP G5EBR3
C	305	THR	-	linker	UNP G5EBR3
C	340	HIS	-	expression tag	UNP G5EBR3
C	341	HIS	-	expression tag	UNP G5EBR3
C	342	HIS	-	expression tag	UNP G5EBR3
C	343	HIS	-	expression tag	UNP G5EBR3
C	344	HIS	-	expression tag	UNP G5EBR3
C	345	HIS	-	expression tag	UNP G5EBR3
C	346	HIS	-	expression tag	UNP G5EBR3
C	347	HIS	-	expression tag	UNP G5EBR3
D	303	ALA	-	linker	UNP G5EBR3
D	304	GLY	-	linker	UNP G5EBR3
D	305	THR	-	linker	UNP G5EBR3
D	340	HIS	-	expression tag	UNP G5EBR3
D	341	HIS	-	expression tag	UNP G5EBR3
D	342	HIS	-	expression tag	UNP G5EBR3
D	343	HIS	-	expression tag	UNP G5EBR3
D	344	HIS	-	expression tag	UNP G5EBR3
D	345	HIS	-	expression tag	UNP G5EBR3
D	346	HIS	-	expression tag	UNP G5EBR3
D	347	HIS	-	expression tag	UNP G5EBR3
E	303	ALA	-	linker	UNP G5EBR3
E	304	GLY	-	linker	UNP G5EBR3
E	305	THR	-	linker	UNP G5EBR3
E	340	HIS	-	expression tag	UNP G5EBR3
E	341	HIS	-	expression tag	UNP G5EBR3
E	342	HIS	-	expression tag	UNP G5EBR3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	343	HIS	-	expression tag	UNP G5EBR3
E	344	HIS	-	expression tag	UNP G5EBR3
E	345	HIS	-	expression tag	UNP G5EBR3
E	346	HIS	-	expression tag	UNP G5EBR3
E	347	HIS	-	expression tag	UNP G5EBR3
P	303	ALA	-	linker	UNP G5EBR3
P	304	GLY	-	linker	UNP G5EBR3
P	305	THR	-	linker	UNP G5EBR3
P	340	HIS	-	expression tag	UNP G5EBR3
P	341	HIS	-	expression tag	UNP G5EBR3
P	342	HIS	-	expression tag	UNP G5EBR3
P	343	HIS	-	expression tag	UNP G5EBR3
P	344	HIS	-	expression tag	UNP G5EBR3
P	345	HIS	-	expression tag	UNP G5EBR3
P	346	HIS	-	expression tag	UNP G5EBR3
P	347	HIS	-	expression tag	UNP G5EBR3
Q	303	ALA	-	linker	UNP G5EBR3
Q	304	GLY	-	linker	UNP G5EBR3
Q	305	THR	-	linker	UNP G5EBR3
Q	340	HIS	-	expression tag	UNP G5EBR3
Q	341	HIS	-	expression tag	UNP G5EBR3
Q	342	HIS	-	expression tag	UNP G5EBR3
Q	343	HIS	-	expression tag	UNP G5EBR3
Q	344	HIS	-	expression tag	UNP G5EBR3
Q	345	HIS	-	expression tag	UNP G5EBR3
Q	346	HIS	-	expression tag	UNP G5EBR3
Q	347	HIS	-	expression tag	UNP G5EBR3
R	303	ALA	-	linker	UNP G5EBR3
R	304	GLY	-	linker	UNP G5EBR3
R	305	THR	-	linker	UNP G5EBR3
R	340	HIS	-	expression tag	UNP G5EBR3
R	341	HIS	-	expression tag	UNP G5EBR3
R	342	HIS	-	expression tag	UNP G5EBR3
R	343	HIS	-	expression tag	UNP G5EBR3
R	344	HIS	-	expression tag	UNP G5EBR3
R	345	HIS	-	expression tag	UNP G5EBR3
R	346	HIS	-	expression tag	UNP G5EBR3
R	347	HIS	-	expression tag	UNP G5EBR3
S	303	ALA	-	linker	UNP G5EBR3
S	304	GLY	-	linker	UNP G5EBR3
S	305	THR	-	linker	UNP G5EBR3
S	340	HIS	-	expression tag	UNP G5EBR3

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Chain	Residue	Modelled	Actual	Comment	Reference
S	341	HIS	-	expression tag	UNP G5EBR3
S	342	HIS	-	expression tag	UNP G5EBR3
S	343	HIS	-	expression tag	UNP G5EBR3
S	344	HIS	-	expression tag	UNP G5EBR3
S	345	HIS	-	expression tag	UNP G5EBR3
S	346	HIS	-	expression tag	UNP G5EBR3
S	347	HIS	-	expression tag	UNP G5EBR3
T	303	ALA	-	linker	UNP G5EBR3
T	304	GLY	-	linker	UNP G5EBR3
T	305	THR	-	linker	UNP G5EBR3
T	340	HIS	-	expression tag	UNP G5EBR3
T	341	HIS	-	expression tag	UNP G5EBR3
T	342	HIS	-	expression tag	UNP G5EBR3
T	343	HIS	-	expression tag	UNP G5EBR3
T	344	HIS	-	expression tag	UNP G5EBR3
T	345	HIS	-	expression tag	UNP G5EBR3
T	346	HIS	-	expression tag	UNP G5EBR3
T	347	HIS	-	expression tag	UNP G5EBR3

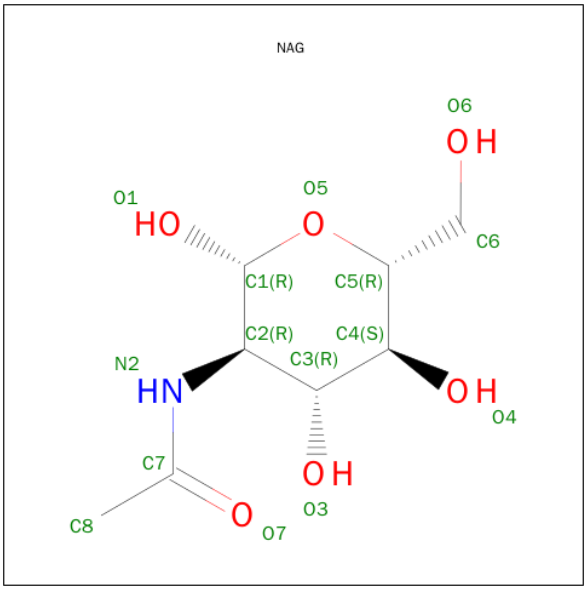
- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	222	Total	C	N	O	S	0	0	0
			1693	1073	277	335	8			
2	G	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	H	223	Total	C	N	O	S	0	0	0
			1701	1077	278	338	8			
2	U	221	Total	C	N	O	S	0	0	0
			1682	1067	273	334	8			
2	V	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	W	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	X	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	Y	221	Total	C	N	O	S	0	0	0
			1682	1067	273	334	8			
2	J	223	Total	C	N	O	S	0	0	0
			1701	1077	278	338	8			
2	I	222	Total	C	N	O	S	0	0	0
			1693	1073	277	335	8			

- Molecule 3 is a protein called Mouse monoclonal Fab fragment, light chain.

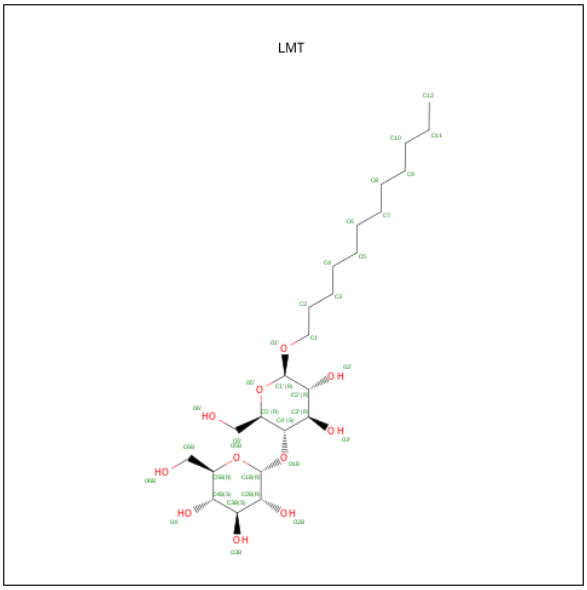
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	212	Total	C	N	O	S	0	0	0
			1606	1008	271	321	6			
3	L	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	N	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	O	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	Z	215	Total	C	N	O	S	0	0	0
			1626	1018	274	327	7			
3	f	214	Total	C	N	O	S	0	0	0
			1620	1015	273	325	7			
3	g	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	h	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	i	214	Total	C	N	O	S	0	0	0
			1620	1015	273	325	7			
3	M	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	S	1	Total	C	N	O	0	0
			14	8	1	5		
4	T	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			23	12	11		

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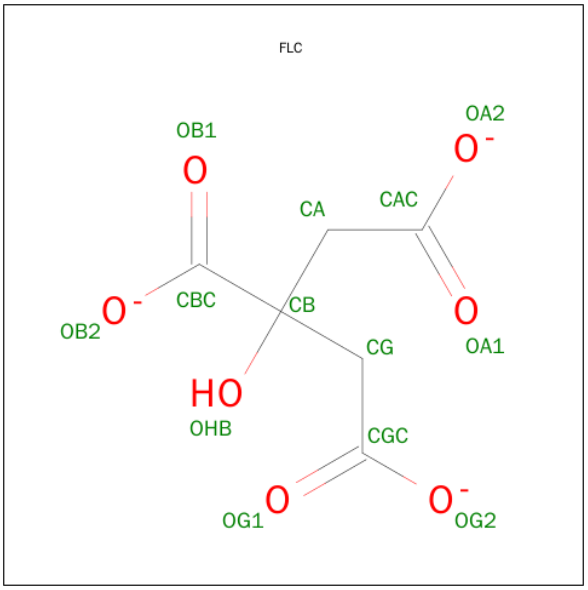
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 23 12 11	0	0
5	C	1	Total C O 23 12 11	0	0
5	D	1	Total C O 23 12 11	0	0
5	E	1	Total C O 23 12 11	0	0
5	P	1	Total C O 23 12 11	0	0
5	Q	1	Total C O 23 12 11	0	0
5	R	1	Total C O 23 12 11	0	0
5	S	1	Total C O 23 12 11	0	0
5	T	1	Total C O 25 14 11	0	0

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 6 7	0	0
6	T	1	Total C O 13 6 7	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

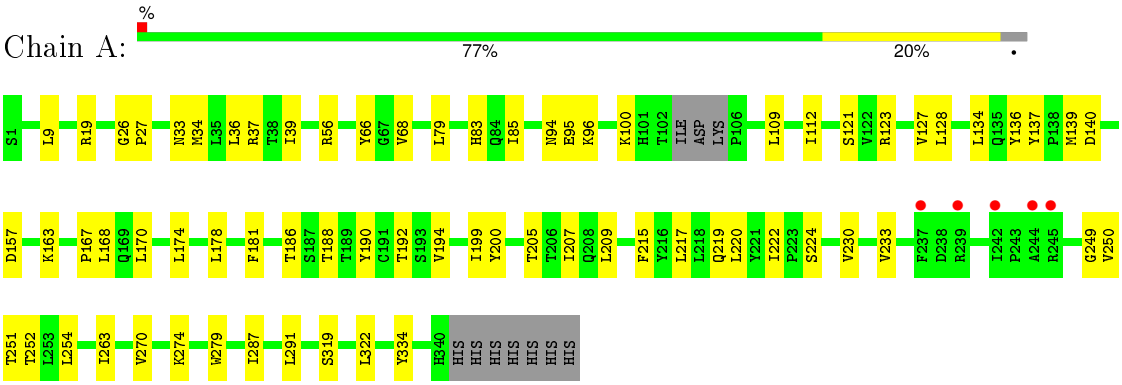
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	P	2	Total Cl 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

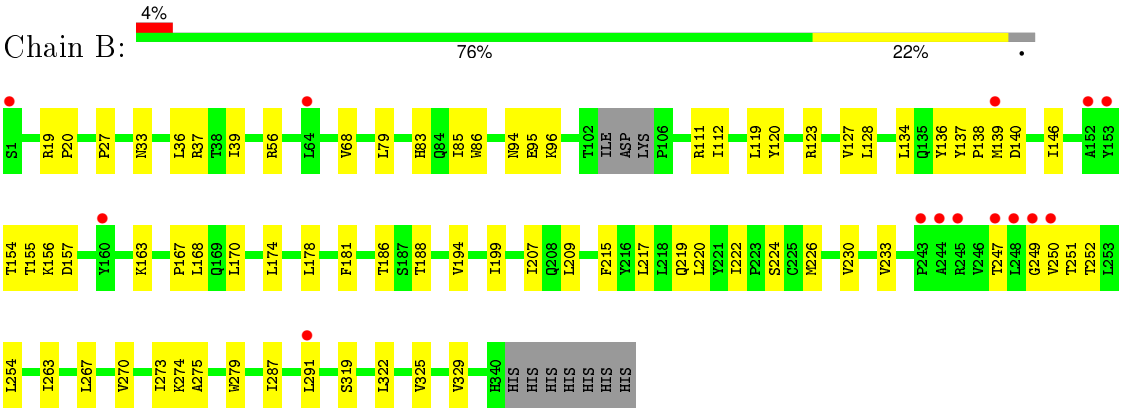
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain A:



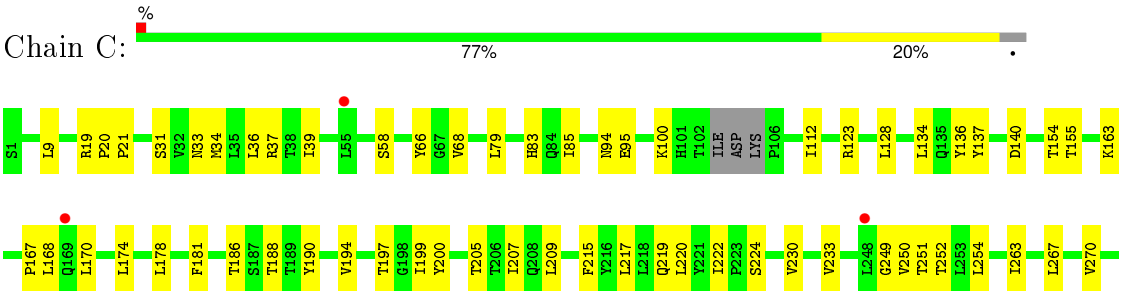
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain B:



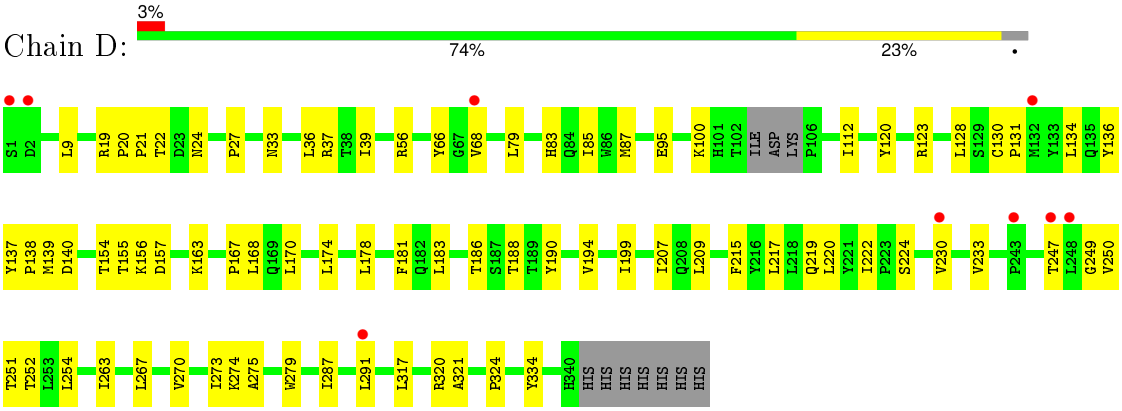
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain C:



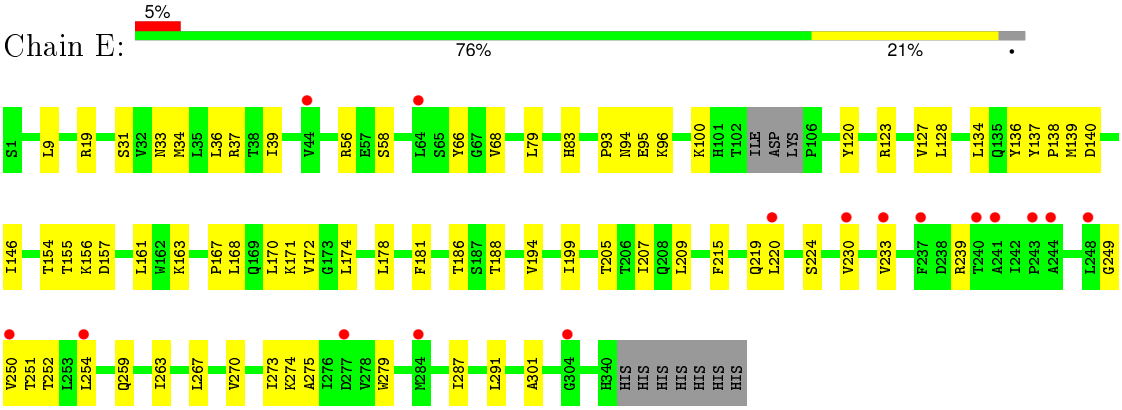
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain D:



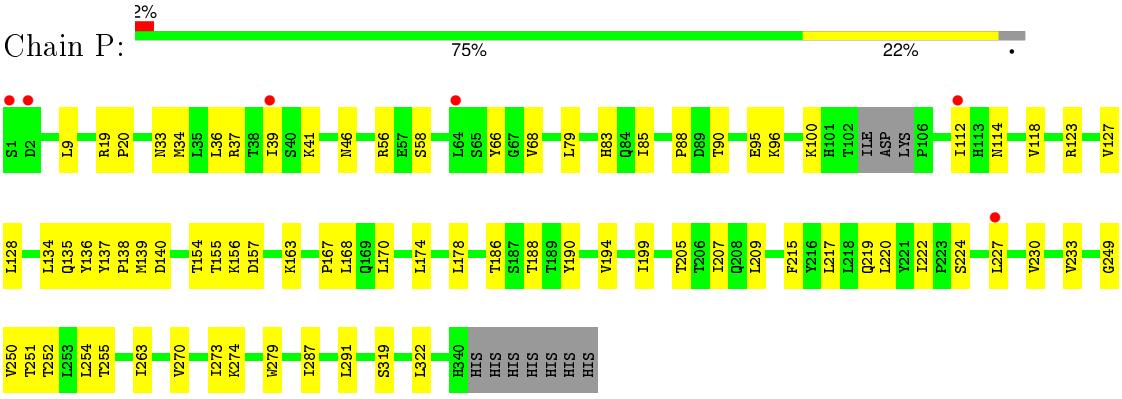
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain E:



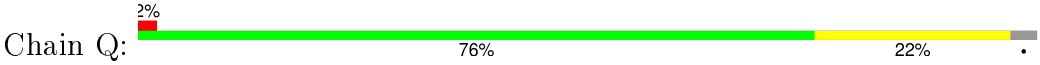
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

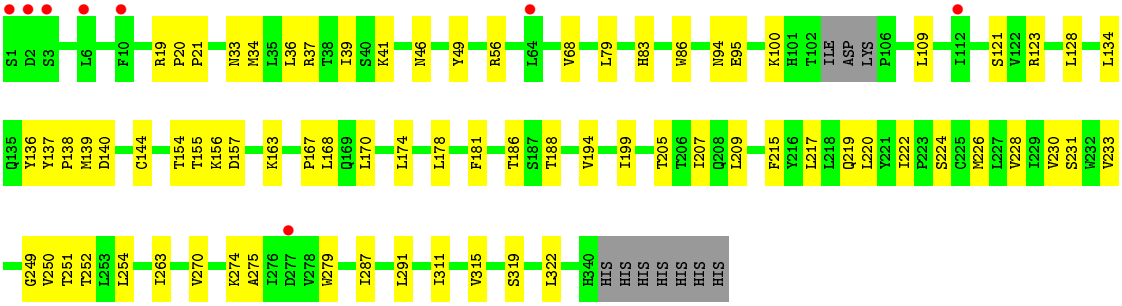
Chain P:



• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

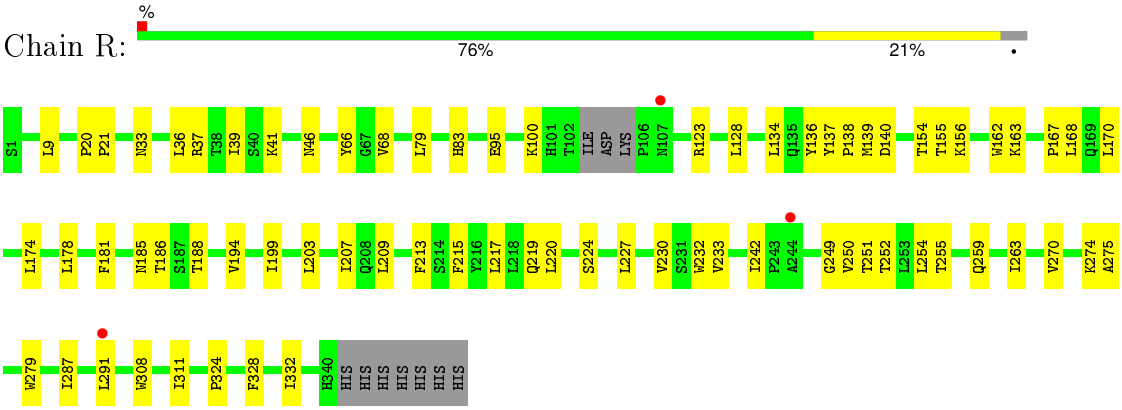
Chain Q:





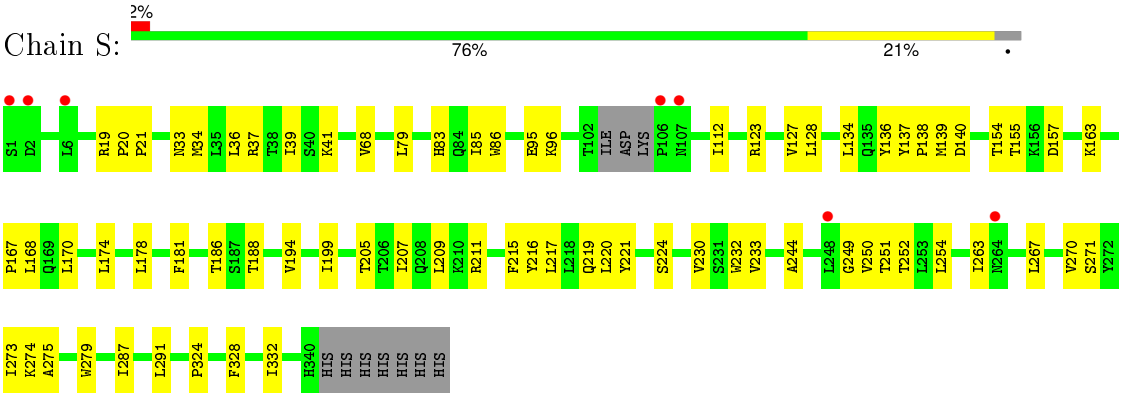
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain R:



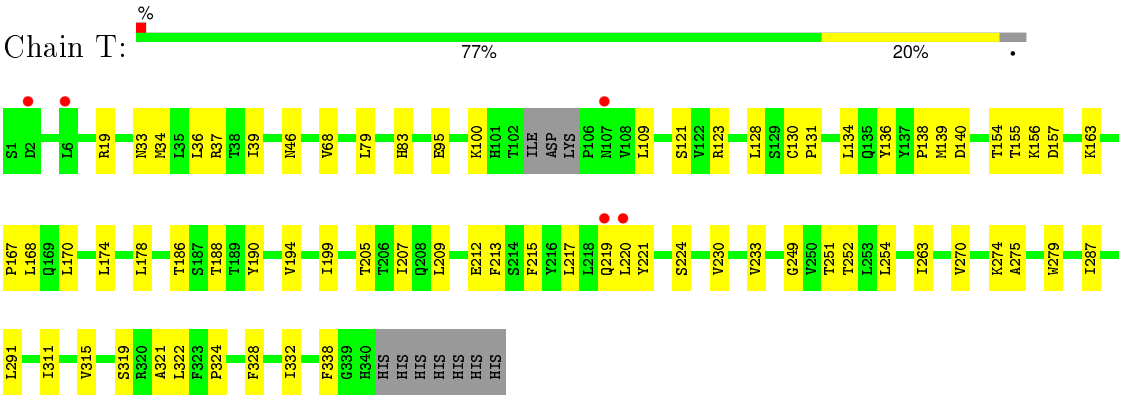
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain S:



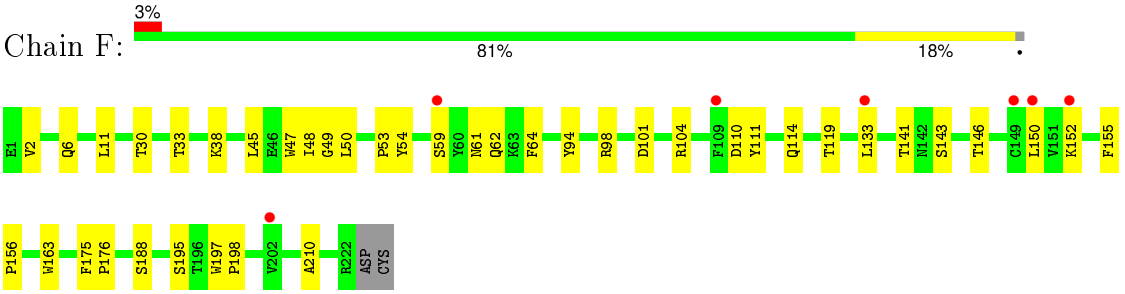
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain T:



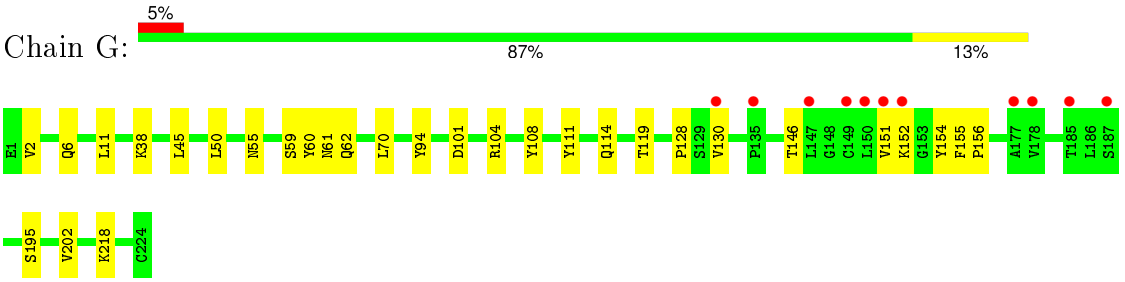
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain F:



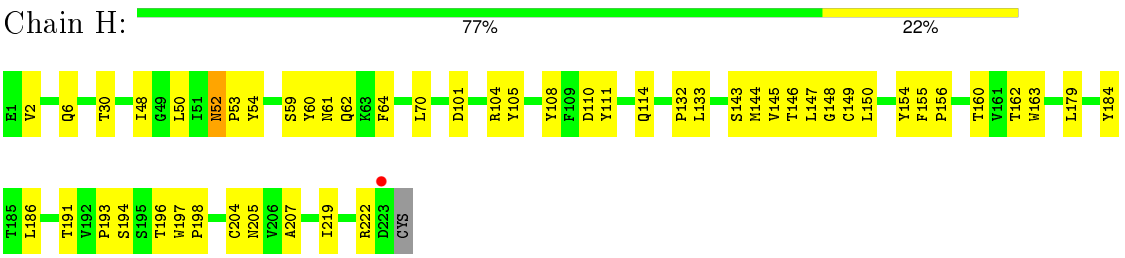
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain G:



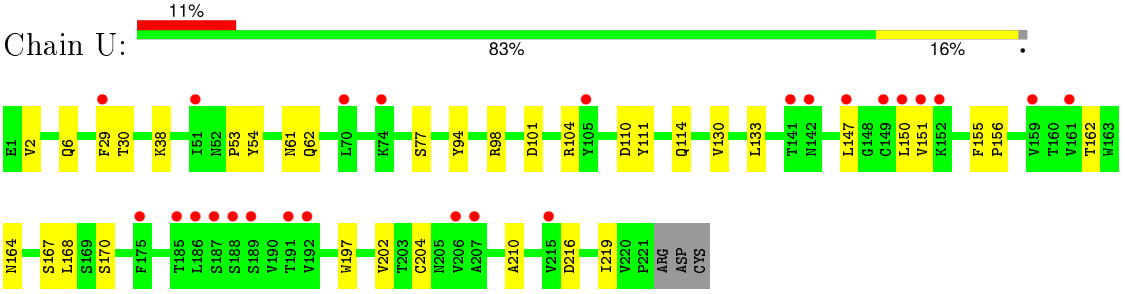
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain H:



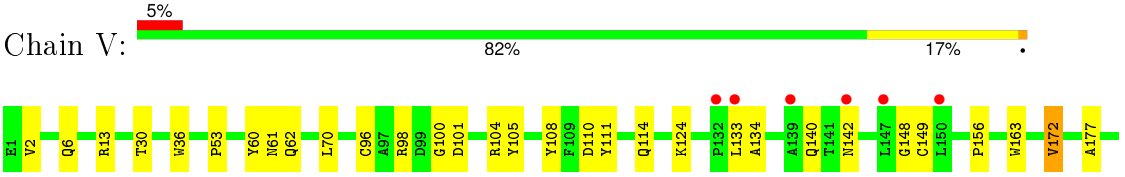
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain U:



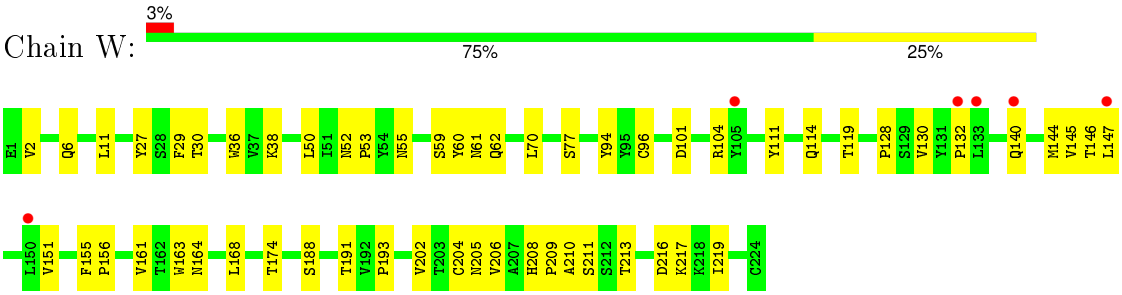
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain V:



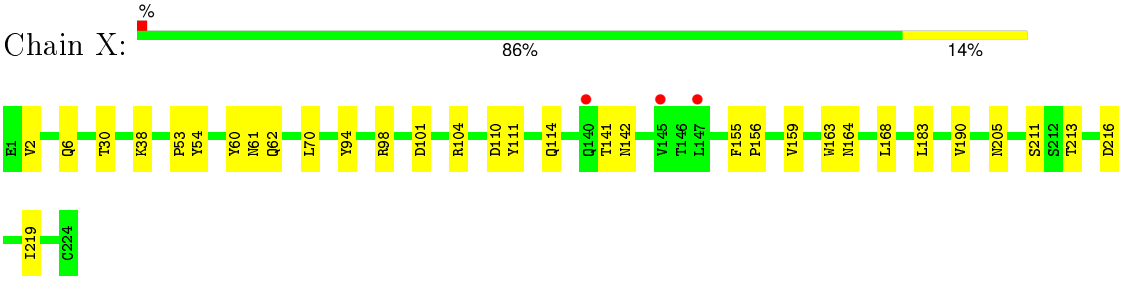
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain W:



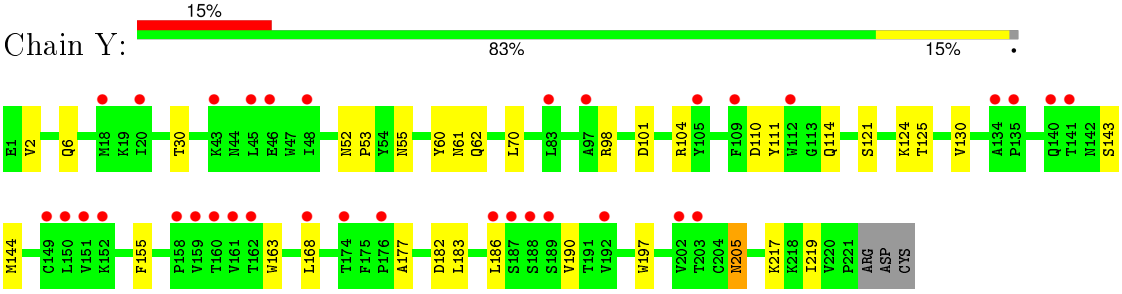
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain X:



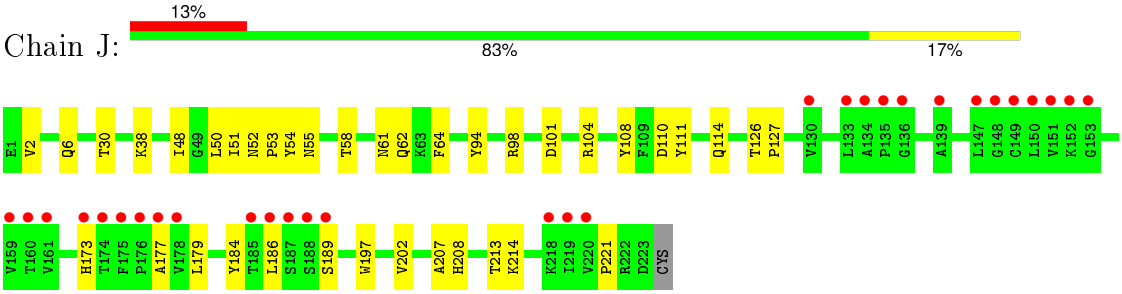
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain Y:



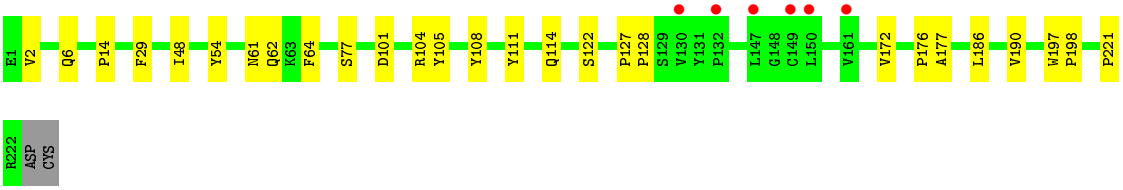
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain J:

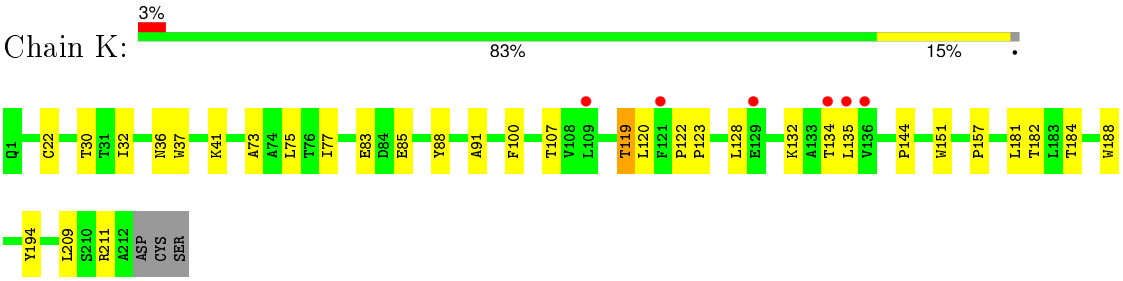


• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

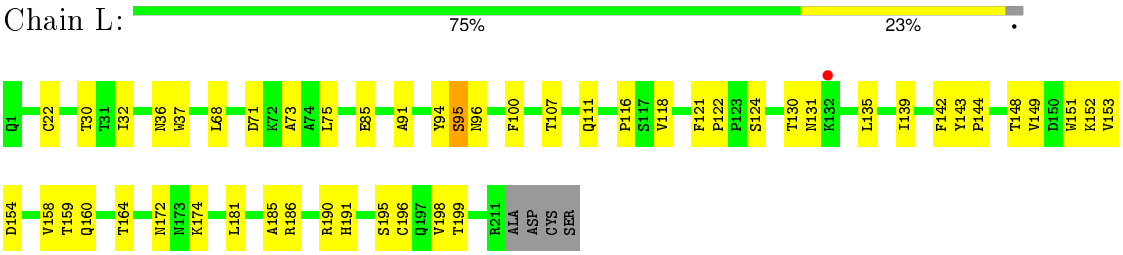
Chain I:



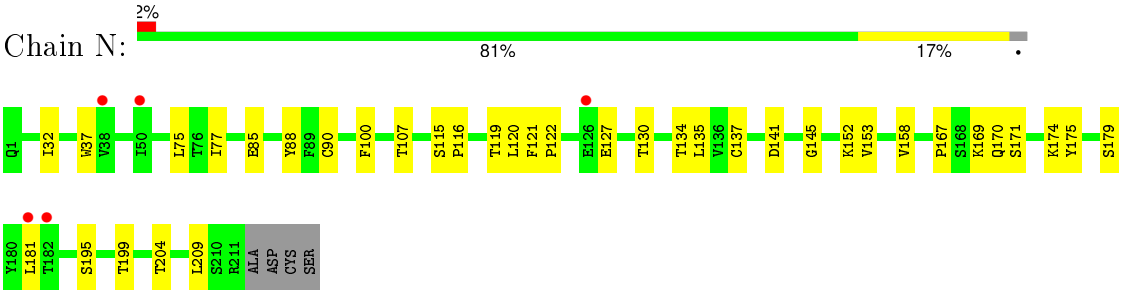
• Molecule 3: Mouse monoclonal Fab fragment, light chain



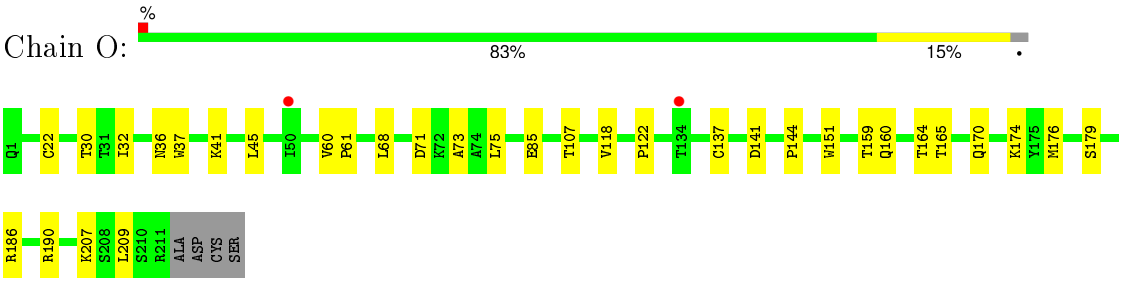
• Molecule 3: Mouse monoclonal Fab fragment, light chain



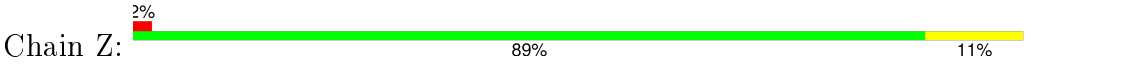
• Molecule 3: Mouse monoclonal Fab fragment, light chain

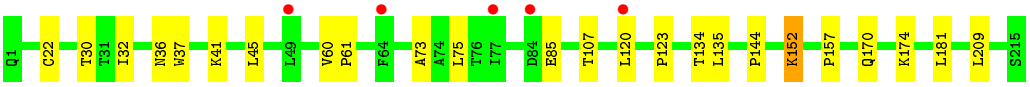


• Molecule 3: Mouse monoclonal Fab fragment, light chain



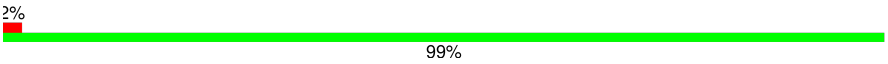
• Molecule 3: Mouse monoclonal Fab fragment, light chain

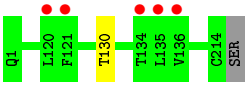




• Molecule 3: Mouse monoclonal Fab fragment, light chain

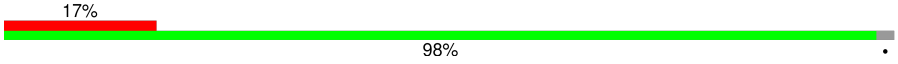
Chain f:

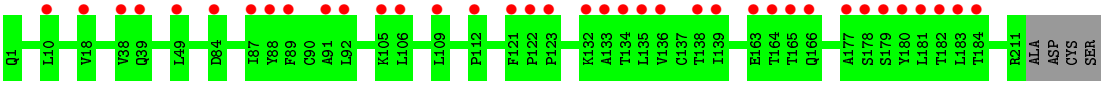




• Molecule 3: Mouse monoclonal Fab fragment, light chain

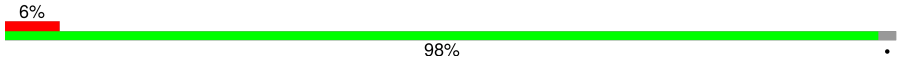
Chain g:

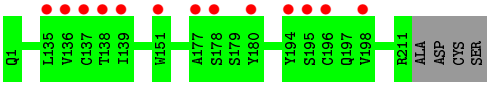




• Molecule 3: Mouse monoclonal Fab fragment, light chain

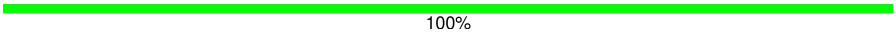
Chain h:





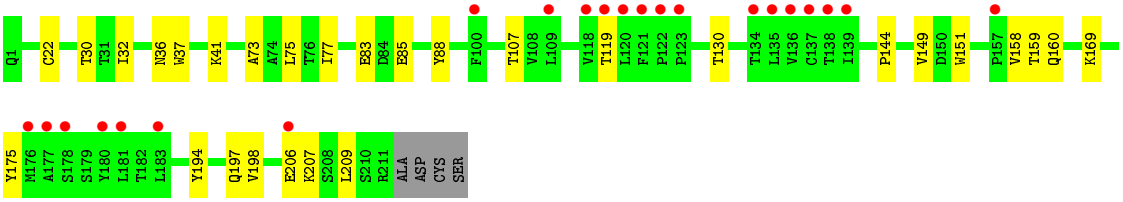
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain i:



• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	455.81Å 195.68Å 196.18Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	58.44 – 3.60 58.44 – 3.60	Depositor EDS
% Data completeness (in resolution range)	88.3 (58.44-3.60) 88.4 (58.44-3.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.261 , 0.283 0.285 , 0.305	Depositor DCC
R_{free} test set	8783 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	121.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 89.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	2 of 175651 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	60408	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, LMT, NAG, CL

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	0.28	0/2767	0.45	0/3776
1	B	0.27	0/2767	0.45	0/3776
1	C	0.28	0/2767	0.46	0/3776
1	D	0.28	0/2767	0.45	0/3776
1	E	0.27	0/2767	0.44	0/3776
1	P	0.29	0/2767	0.46	0/3776
1	Q	0.30	0/2767	0.47	0/3776
1	R	0.30	0/2767	0.47	0/3776
1	S	0.31	0/2767	0.48	0/3776
1	T	0.30	0/2767	0.47	0/3776
2	F	0.25	0/1739	0.43	0/2374
2	G	0.25	0/1753	0.42	0/2393
2	H	0.28	0/1747	0.45	0/2385
2	I	0.25	0/1739	0.43	0/2374
2	J	0.27	0/1747	0.45	0/2385
2	U	0.24	0/1728	0.43	0/2360
2	V	0.25	0/1753	0.44	0/2393
2	W	0.27	0/1753	0.44	0/2393
2	X	0.26	0/1753	0.45	0/2393
2	Y	0.24	0/1728	0.44	0/2360
3	K	0.27	0/1644	0.45	0/2247
3	L	0.30	0/1639	0.48	0/2240
3	M	0.25	0/1639	0.46	0/2240
3	N	0.24	0/1639	0.43	0/2240
3	O	0.25	0/1639	0.44	0/2240
3	Z	0.25	0/1664	0.45	0/2274
3	f	0.28	0/1658	0.45	0/2266
3	g	0.24	0/1639	0.45	0/2240
3	h	0.25	0/1639	0.44	0/2240
3	i	0.28	0/1658	0.46	0/2266
All	All	0.27	0/61568	0.45	0/84063

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2695	0	2691	51	0
1	B	2695	0	2691	49	0
1	C	2695	0	2691	50	0
1	D	2695	0	2691	60	0
1	E	2695	0	2691	56	0
1	P	2695	0	2691	52	0
1	Q	2695	0	2691	56	0
1	R	2695	0	2691	53	0
1	S	2695	0	2691	53	0
1	T	2695	0	2691	53	0
2	F	1693	0	1645	30	0
2	G	1707	0	1654	21	0
2	H	1701	0	1649	36	0
2	I	1693	0	1645	19	0
2	J	1701	0	1649	25	0
2	U	1682	0	1632	20	0
2	V	1707	0	1653	25	0
2	W	1707	0	1653	36	0
2	X	1707	0	1653	19	0
2	Y	1682	0	1632	21	0
3	K	1606	0	1560	22	0
3	L	1601	0	1555	30	0
3	M	1601	0	1555	17	0
3	N	1601	0	1555	26	0
3	O	1601	0	1555	21	0
3	Z	1626	0	1573	15	0
3	f	1620	0	1568	0	0
3	g	1601	0	1555	0	0
3	h	1601	0	1555	0	0
3	i	1620	0	1568	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	P	14	0	13	0	0
4	Q	14	0	13	0	0
4	R	14	0	13	1	0
4	S	14	0	13	0	0
4	T	14	0	13	0	0
5	A	23	0	21	0	0
5	B	23	0	21	1	0
5	C	23	0	21	0	0
5	D	23	0	21	0	0
5	E	23	0	21	0	0
5	P	23	0	21	0	0
5	Q	23	0	21	0	0
5	R	23	0	21	0	0
5	S	23	0	21	0	0
5	T	25	0	23	0	0
6	A	13	0	5	0	0
6	T	13	0	5	1	0
7	P	2	0	0	0	0
All	All	60408	0	59326	827	0

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 8.

All (827) 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)
3:M:107:THR:HG21	3:M:144:PRO:HB3	1.66	0.77
1:P:254:LEU:HD11	1:Q:254:LEU:HD22	1.67	0.74
1:S:254:LEU:HD11	1:T:254:LEU:HD22	1.69	0.73
2:Y:130:VAL:HB	2:Y:217:LYS:HG3	1.72	0.72
2:F:6:GLN:H	2:F:114:GLN:HE22	1.37	0.72
3:L:131:ASN:HA	3:L:185:ALA:HB2	1.72	0.72
2:H:144:MET:HG2	2:H:193:PRO:HA	1.69	0.72
1:R:254:LEU:HD11	1:S:254:LEU:HD22	1.72	0.71
1:A:254:LEU:HD22	1:E:254:LEU:HD11	1.72	0.70
1:B:254:LEU:HD11	1:C:254:LEU:HD22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:101:ASP:HB3	2:G:104:ARG:HG3	1.74	0.70
1:T:33:ASN:HB2	1:T:163:LYS:HD2	1.74	0.70
1:A:37:ARG:HH21	1:A:123:ARG:CZ	2.04	0.69
1:P:254:LEU:HD22	1:T:254:LEU:HD11	1.75	0.68
3:K:122:PRO:HG3	3:K:209:LEU:HD13	1.73	0.68
1:D:170:LEU:HD23	1:D:174:LEU:HD22	1.75	0.68
2:V:6:GLN:H	2:V:114:GLN:HE22	1.41	0.68
1:D:33:ASN:HB2	1:D:163:LYS:HD2	1.76	0.68
1:B:167:PRO:HB2	1:B:188:THR:HG21	1.76	0.67
1:C:33:ASN:HB2	1:C:163:LYS:HD2	1.76	0.67
2:Y:6:GLN:H	2:Y:114:GLN:HE22	1.42	0.67
1:E:36:LEU:HD13	1:E:168:LEU:HD11	1.76	0.67
1:A:254:LEU:HD11	1:B:254:LEU:HD22	1.77	0.67
2:I:6:GLN:H	2:I:114:GLN:HE22	1.41	0.66
1:Q:254:LEU:HD11	1:R:254:LEU:HD22	1.76	0.66
3:Z:107:THR:HG21	3:Z:144:PRO:HB3	1.77	0.66
1:P:136:TYR:O	1:P:140:ASP:HB3	1.96	0.66
1:E:170:LEU:HD23	1:E:174:LEU:HD22	1.76	0.65
1:T:136:TYR:O	1:T:140:ASP:HB3	1.96	0.65
2:V:177:ALA:HB2	2:V:186:LEU:HD23	1.79	0.65
2:X:6:GLN:H	2:X:114:GLN:HE22	1.42	0.65
1:B:250:VAL:HB	1:C:251:THR:HG21	1.77	0.65
1:A:194:VAL:HG22	1:A:199:ILE:HG23	1.78	0.65
1:A:33:ASN:HB2	1:A:163:LYS:HD2	1.78	0.65
2:J:6:GLN:H	2:J:114:GLN:HE22	1.45	0.64
1:C:254:LEU:HD11	1:D:254:LEU:HD22	1.79	0.64
3:N:141:ASP:HA	3:N:174:LYS:HB3	1.78	0.64
1:C:194:VAL:HG22	1:C:199:ILE:HG23	1.80	0.64
2:J:101:ASP:HB3	2:J:104:ARG:HG3	1.79	0.64
1:R:134:LEU:HD12	1:R:270:VAL:HG11	1.78	0.64
1:R:170:LEU:HD23	1:R:174:LEU:HD22	1.80	0.63
1:R:136:TYR:O	1:R:140:ASP:HB3	1.98	0.63
1:Q:136:TYR:O	1:Q:140:ASP:HB3	1.98	0.63
1:A:36:LEU:HD13	1:A:168:LEU:HD11	1.80	0.63
1:D:36:LEU:HD13	1:D:168:LEU:HD11	1.80	0.63
1:B:220:LEU:HG	1:B:263:ILE:HD12	1.81	0.63
3:L:148:THR:HB	3:L:199:THR:HB	1.81	0.62
1:D:254:LEU:HD11	1:E:254:LEU:HD22	1.81	0.62
1:E:136:TYR:O	1:E:140:ASP:HB3	2.00	0.62
1:S:136:TYR:O	1:S:140:ASP:HB3	1.99	0.62
1:A:136:TYR:O	1:A:140:ASP:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:167:PRO:HB2	1:P:188:THR:HG21	1.80	0.62
1:B:194:VAL:HG22	1:B:199:ILE:HG23	1.81	0.62
2:H:52:ASN:HD22	2:H:54:TYR:H	1.48	0.62
2:V:101:ASP:HB3	2:V:104:ARG:HG3	1.82	0.61
1:B:136:TYR:O	1:B:140:ASP:HB3	1.99	0.61
2:G:6:GLN:H	2:G:114:GLN:HE22	1.47	0.61
2:J:30:THR:HA	2:J:53:PRO:HB2	1.82	0.61
1:T:167:PRO:HB2	1:T:188:THR:HG21	1.82	0.61
1:R:167:PRO:HB2	1:R:188:THR:HG21	1.81	0.61
1:C:136:TYR:O	1:C:140:ASP:HB3	2.00	0.61
2:W:147:LEU:HD22	2:W:219:ILE:HG21	1.82	0.61
2:W:6:GLN:H	2:W:114:GLN:HE22	1.48	0.61
2:W:211:SER:HG	2:W:213:THR:HG1	1.44	0.61
2:X:101:ASP:HB3	2:X:104:ARG:HG3	1.82	0.61
1:A:167:PRO:HB2	1:A:188:THR:HG21	1.81	0.61
1:D:136:TYR:O	1:D:140:ASP:HB3	2.01	0.61
2:H:101:ASP:HB3	2:H:104:ARG:HG3	1.82	0.61
1:R:33:ASN:HB2	1:R:163:LYS:HD2	1.81	0.60
2:J:197:TRP:HE1	2:J:202:VAL:HB	1.66	0.60
2:F:156:PRO:HD2	2:F:210:ALA:HB1	1.84	0.60
1:B:33:ASN:HB2	1:B:163:LYS:HD2	1.83	0.60
3:K:107:THR:HG21	3:K:144:PRO:HB3	1.84	0.60
3:M:194:TYR:HB2	3:M:209:LEU:HB3	1.83	0.60
1:B:39:ILE:HB	1:B:178:LEU:HD11	1.84	0.60
1:C:170:LEU:HD23	1:C:174:LEU:HD22	1.84	0.60
2:W:164:ASN:HD22	2:W:168:LEU:HD13	1.66	0.60
2:Y:101:ASP:HB3	2:Y:104:ARG:HG3	1.84	0.60
2:F:141:THR:HG22	2:F:143:SER:H	1.66	0.59
2:Y:98:ARG:NH2	2:Y:110:ASP:OD2	2.32	0.59
1:T:36:LEU:HD13	1:T:168:LEU:HD11	1.83	0.59
2:I:101:ASP:HB3	2:I:104:ARG:HG3	1.83	0.59
2:V:134:ALA:HB1	2:V:222:ARG:HB2	1.84	0.59
1:A:190:TYR:O	2:H:104:ARG:NH1	2.36	0.59
2:J:98:ARG:NH2	2:J:110:ASP:OD2	2.25	0.59
1:A:251:THR:HG21	1:E:250:VAL:HB	1.85	0.59
1:P:134:LEU:HD12	1:P:270:VAL:HG11	1.84	0.59
1:S:167:PRO:HB2	1:S:188:THR:HG21	1.84	0.58
3:K:22:CYS:HB3	3:K:73:ALA:HB3	1.85	0.58
1:C:190:TYR:O	2:G:104:ARG:NH1	2.36	0.58
1:E:167:PRO:HB2	1:E:188:THR:HG21	1.83	0.58
1:A:170:LEU:HD23	1:A:174:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ILE:HD12	1:C:209:LEU:HD21	1.85	0.58
3:N:153:VAL:HG12	3:N:158:VAL:HG22	1.86	0.58
3:L:85:GLU:HG3	3:L:107:THR:HA	1.86	0.58
1:C:134:LEU:HD12	1:C:270:VAL:HG11	1.85	0.58
3:M:194:TYR:N	3:M:209:LEU:O	2.35	0.58
2:G:146:THR:HB	3:K:119:THR:HG21	1.85	0.58
1:T:134:LEU:HD12	1:T:270:VAL:HG11	1.84	0.58
1:Q:95:GLU:HA	1:Q:128:LEU:HD23	1.85	0.58
1:D:250:VAL:HB	1:E:251:THR:HG21	1.86	0.58
1:A:79:LEU:HD11	1:A:83:HIS:HB2	1.86	0.58
1:Q:138:PRO:HD2	1:Q:139:MET:HE3	1.86	0.58
2:Y:177:ALA:HB2	2:Y:186:LEU:HD23	1.85	0.57
2:Y:197:TRP:HE1	2:Y:219:ILE:HG12	1.68	0.57
1:Q:134:LEU:HD12	1:Q:270:VAL:HG11	1.85	0.57
1:B:36:LEU:HD13	1:B:168:LEU:HD11	1.86	0.57
1:B:170:LEU:HD23	1:B:174:LEU:HD22	1.84	0.57
3:N:37:TRP:CE2	3:N:75:LEU:HB2	2.40	0.57
1:D:154:THR:OG1	1:D:155:THR:N	2.38	0.57
1:B:207:ILE:HD12	1:B:209:LEU:HD21	1.86	0.57
1:P:170:LEU:HD23	1:P:174:LEU:HD22	1.87	0.57
1:E:39:ILE:HB	1:E:178:LEU:HD11	1.86	0.57
1:Q:170:LEU:HD23	1:Q:174:LEU:HD22	1.87	0.57
1:Q:167:PRO:HB2	1:Q:188:THR:HG21	1.87	0.57
1:Q:39:ILE:HB	1:Q:178:LEU:HD11	1.85	0.57
1:Q:36:LEU:HD13	1:Q:168:LEU:HD11	1.86	0.56
1:T:170:LEU:HD23	1:T:174:LEU:HD22	1.87	0.56
2:U:6:GLN:H	2:U:114:GLN:HE22	1.52	0.56
1:E:134:LEU:HD12	1:E:270:VAL:HG11	1.86	0.56
1:S:33:ASN:HB2	1:S:163:LYS:HD2	1.87	0.56
3:M:22:CYS:HB3	3:M:73:ALA:HB3	1.86	0.56
1:Q:220:LEU:HG	1:Q:263:ILE:HD12	1.86	0.56
2:U:130:VAL:HG22	2:U:151:VAL:HG22	1.87	0.56
1:R:46:ASN:ND2	1:S:41:LYS:HE2	2.19	0.56
2:J:52:ASN:ND2	2:J:55:ASN:HD22	2.04	0.56
1:P:194:VAL:O	2:W:55:ASN:ND2	2.38	0.56
2:W:161:VAL:HG22	2:W:206:VAL:HG22	1.87	0.56
1:P:36:LEU:HD13	1:P:168:LEU:HD11	1.87	0.56
3:K:134:THR:HG22	3:K:182:THR:HA	1.87	0.56
1:C:36:LEU:HD13	1:C:168:LEU:HD11	1.88	0.56
3:K:37:TRP:CE2	3:K:75:LEU:HB2	2.41	0.56
2:F:101:ASP:HB3	2:F:104:ARG:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:33:ASN:HB2	1:P:163:LYS:HD2	1.87	0.56
2:H:6:GLN:H	2:H:114:GLN:HE22	1.53	0.56
1:T:154:THR:OG1	1:T:155:THR:N	2.37	0.56
1:D:39:ILE:HB	1:D:178:LEU:HD11	1.88	0.55
1:D:134:LEU:HD12	1:D:270:VAL:HG11	1.88	0.55
1:E:154:THR:OG1	1:E:155:THR:N	2.35	0.55
2:J:173:HIS:HB2	2:J:189:SER:HB2	1.88	0.55
2:J:208:HIS:N	2:J:213:THR:O	2.26	0.55
1:B:134:LEU:HD12	1:B:270:VAL:HG11	1.89	0.55
2:W:101:ASP:HB3	2:W:104:ARG:HG3	1.89	0.55
2:H:108:TYR:HA	3:L:36:ASN:HD21	1.72	0.55
1:P:39:ILE:HB	1:P:178:LEU:HD11	1.88	0.55
3:L:116:PRO:HB3	3:L:142:PHE:HB3	1.88	0.55
1:C:37:ARG:HE	1:C:123:ARG:HD3	1.72	0.55
1:P:274:LYS:HZ2	1:Q:215:PHE:HE1	1.55	0.55
2:X:205:ASN:ND2	2:X:216:ASP:OD1	2.40	0.55
1:B:252:THR:HG22	1:B:287:ILE:HD13	1.89	0.55
1:C:167:PRO:HB2	1:C:188:THR:HG21	1.88	0.55
1:E:95:GLU:HA	1:E:128:LEU:HD23	1.89	0.55
1:R:79:LEU:HD11	1:R:83:HIS:HB2	1.88	0.54
1:T:194:VAL:HG22	1:T:199:ILE:HG23	1.89	0.54
3:N:145:GLY:HA3	3:N:175:TYR:HD2	1.71	0.54
3:M:85:GLU:HG3	3:M:107:THR:HA	1.88	0.54
1:B:95:GLU:HA	1:B:128:LEU:HD23	1.89	0.54
1:P:249:GLY:HA3	1:P:291:LEU:HD13	1.90	0.54
1:R:154:THR:OG1	1:R:155:THR:N	2.39	0.54
1:S:95:GLU:HA	1:S:128:LEU:HD23	1.90	0.54
1:T:138:PRO:HD2	1:T:139:MET:HE3	1.90	0.54
1:R:36:LEU:HD13	1:R:168:LEU:HD11	1.88	0.54
1:R:194:VAL:HG22	1:R:199:ILE:HG23	1.90	0.54
1:P:41:LYS:HE2	1:T:46:ASN:ND2	2.23	0.54
1:S:249:GLY:HA3	1:S:291:LEU:HD13	1.89	0.54
1:E:34:MET:SD	1:E:205:THR:HG21	2.47	0.54
1:T:37:ARG:HH21	1:T:123:ARG:CZ	2.21	0.54
2:F:61:ASN:OD1	2:F:62:GLN:N	2.41	0.54
3:O:122:PRO:HB3	3:O:209:LEU:HD21	1.90	0.54
3:O:165:THR:HB	2:I:176:PRO:HG2	1.90	0.54
2:H:133:LEU:HD11	2:H:150:LEU:HB2	1.88	0.54
2:J:108:TYR:HA	3:M:36:ASN:HD21	1.72	0.54
1:B:154:THR:OG1	1:B:155:THR:N	2.41	0.54
2:U:101:ASP:HB3	2:U:104:ARG:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:217:LEU:O	1:Q:222:ILE:HG12	2.07	0.54
3:N:199:THR:HG23	3:N:204:THR:HB	1.90	0.54
1:A:134:LEU:HD12	1:A:270:VAL:HG11	1.89	0.53
1:T:220:LEU:HG	1:T:263:ILE:HD12	1.90	0.53
1:E:33:ASN:HB2	1:E:163:LYS:HD2	1.89	0.53
1:C:252:THR:HG22	1:C:287:ILE:HD13	1.91	0.53
1:Q:224:SER:HB2	1:Q:279:TRP:CZ3	2.43	0.53
2:X:60:TYR:HE1	2:X:70:LEU:HG	1.73	0.53
2:I:172:VAL:HA	2:I:190:VAL:HG22	1.90	0.53
1:R:39:ILE:HB	1:R:178:LEU:HD11	1.90	0.53
3:L:94:TYR:O	3:L:96:ASN:N	2.38	0.53
1:T:194:VAL:O	2:Y:55:ASN:ND2	2.42	0.53
3:N:169:LYS:HA	3:N:175:TYR:HD1	1.74	0.53
2:V:156:PRO:HD2	2:V:210:ALA:HB1	1.91	0.53
1:C:194:VAL:O	2:G:55:ASN:ND2	2.41	0.53
1:T:230:VAL:O	1:T:233:VAL:HG22	2.09	0.53
1:S:134:LEU:HD12	1:S:270:VAL:HG11	1.90	0.53
3:M:149:VAL:HG22	3:M:198:VAL:HG12	1.90	0.53
1:D:254:LEU:HD12	1:E:251:THR:HG23	1.91	0.53
1:Q:168:LEU:HD23	1:Q:186:THR:HB	1.90	0.53
1:D:249:GLY:HA3	1:D:291:LEU:HD13	1.91	0.53
1:E:168:LEU:HD23	1:E:186:THR:HB	1.91	0.53
1:E:207:ILE:HD12	1:E:209:LEU:HD21	1.90	0.53
2:W:128:PRO:HD3	2:W:208:HIS:ND1	2.24	0.53
2:H:148:GLY:HA2	2:H:163:TRP:HH2	1.73	0.52
2:F:48:ILE:HG12	2:F:64:PHE:CE2	2.44	0.52
3:O:37:TRP:CE2	3:O:75:LEU:HB2	2.44	0.52
1:T:39:ILE:HB	1:T:178:LEU:HD11	1.92	0.52
1:R:252:THR:HG22	1:R:287:ILE:HD13	1.90	0.52
2:I:177:ALA:HB2	2:I:186:LEU:HB2	1.90	0.52
1:T:190:TYR:O	2:Y:104:ARG:NH1	2.42	0.52
1:P:194:VAL:HG22	1:P:199:ILE:HG23	1.92	0.52
2:G:108:TYR:HA	3:K:36:ASN:HD21	1.75	0.52
3:K:85:GLU:HG3	3:K:107:THR:HA	1.90	0.52
1:P:250:VAL:HB	1:Q:251:THR:HG21	1.91	0.52
1:P:154:THR:OG1	1:P:155:THR:N	2.43	0.52
1:R:37:ARG:HH21	1:R:123:ARG:CZ	2.23	0.52
1:D:220:LEU:HG	1:D:263:ILE:HD12	1.91	0.52
1:C:254:LEU:HD12	1:D:251:THR:HG23	1.92	0.52
2:X:60:TYR:CE1	2:X:70:LEU:HG	2.44	0.52
2:I:61:ASN:OD1	2:I:62:GLN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:37:TRP:CE2	3:Z:75:LEU:HB2	2.45	0.52
2:X:211:SER:HG	2:X:213:THR:HG1	1.50	0.52
1:R:224:SER:HB2	1:R:279:TRP:CZ3	2.45	0.52
1:C:95:GLU:HA	1:C:128:LEU:HD23	1.92	0.52
1:D:37:ARG:HH21	1:D:123:ARG:CZ	2.23	0.52
1:T:34:MET:SD	1:T:205:THR:HG21	2.50	0.52
3:Z:30:THR:OG1	3:Z:32:ILE:HG12	2.10	0.51
1:S:168:LEU:HD23	1:S:186:THR:HB	1.92	0.51
1:A:95:GLU:HA	1:A:128:LEU:HD23	1.92	0.51
1:S:224:SER:HB2	1:S:279:TRP:CZ3	2.45	0.51
3:K:151:TRP:O	3:K:157:PRO:HA	2.10	0.51
1:C:79:LEU:HD11	1:C:83:HIS:HB2	1.92	0.51
1:D:207:ILE:HD12	1:D:209:LEU:HD21	1.91	0.51
1:S:274:LYS:NZ	1:T:215:PHE:HE1	2.09	0.51
1:P:95:GLU:HA	1:P:128:LEU:HD23	1.92	0.51
3:L:22:CYS:HB3	3:L:73:ALA:HB3	1.93	0.51
2:I:6:GLN:N	2:I:114:GLN:HE22	2.07	0.51
1:R:168:LEU:HD23	1:R:186:THR:HB	1.93	0.51
1:Q:249:GLY:HA3	1:Q:291:LEU:HD13	1.91	0.51
2:X:141:THR:OG1	2:X:142:ASN:N	2.44	0.51
1:R:230:VAL:O	1:R:233:VAL:HG22	2.10	0.51
2:Y:124:LYS:HG2	2:Y:125:THR:H	1.76	0.51
1:B:249:GLY:HA3	1:B:291:LEU:HD13	1.92	0.51
1:E:249:GLY:HA3	1:E:291:LEU:HD13	1.93	0.51
3:L:153:VAL:HG12	3:L:158:VAL:HG22	1.92	0.51
1:C:168:LEU:HD23	1:C:186:THR:HB	1.93	0.51
1:Q:33:ASN:HB2	1:Q:163:LYS:HD2	1.93	0.51
2:Y:163:TRP:HB2	2:Y:168:LEU:HB2	1.92	0.51
2:H:148:GLY:HA2	2:H:163:TRP:CH2	2.46	0.50
2:H:163:TRP:CZ3	2:H:204:CYS:HB3	2.46	0.50
1:B:79:LEU:HD11	1:B:83:HIS:HB2	1.93	0.50
3:N:85:GLU:HG3	3:N:107:THR:HA	1.94	0.50
2:W:36:TRP:CZ3	2:W:96:CYS:HB3	2.46	0.50
1:T:168:LEU:HD23	1:T:186:THR:HB	1.91	0.50
1:T:37:ARG:HE	1:T:123:ARG:HD3	1.76	0.50
1:A:220:LEU:HG	1:A:263:ILE:HD12	1.93	0.50
2:X:6:GLN:N	2:X:114:GLN:HE22	2.08	0.50
1:P:274:LYS:NZ	1:Q:215:PHE:HE1	2.08	0.50
2:V:61:ASN:OD1	2:V:62:GLN:N	2.45	0.50
1:P:230:VAL:O	1:P:233:VAL:HG22	2.12	0.50
1:B:168:LEU:HD23	1:B:186:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:170:LEU:O	2:X:54:TYR:OH	2.28	0.50
1:S:220:LEU:HG	1:S:263:ILE:HD12	1.93	0.50
1:P:215:PHE:HE1	1:T:274:LYS:NZ	2.10	0.50
1:E:252:THR:HG22	1:E:287:ILE:HD13	1.92	0.50
1:A:34:MET:SD	1:A:205:THR:HG21	2.51	0.50
2:F:152:LYS:NZ	3:N:127:GLU:OE1	2.43	0.50
1:Q:46:ASN:ND2	1:R:41:LYS:HE2	2.26	0.50
1:C:170:LEU:O	2:F:54:TYR:OH	2.23	0.50
1:C:37:ARG:HH21	1:C:123:ARG:CZ	2.24	0.50
1:S:181:PHE:HB3	1:S:209:LEU:HB3	1.94	0.50
3:M:37:TRP:CE2	3:M:75:LEU:HB2	2.47	0.50
1:Q:274:LYS:NZ	1:R:215:PHE:HE1	2.09	0.50
1:P:252:THR:HG22	1:P:287:ILE:HD13	1.93	0.50
1:D:167:PRO:HB2	1:D:188:THR:HG21	1.93	0.50
1:B:19:ARG:HH11	1:B:157:ASP:HA	1.76	0.50
1:T:252:THR:HG22	1:T:287:ILE:HD13	1.93	0.50
1:S:36:LEU:HD13	1:S:168:LEU:HD11	1.94	0.49
2:U:98:ARG:NH2	2:U:110:ASP:OD2	2.38	0.49
3:L:143:TYR:HB2	3:L:174:LYS:HG3	1.93	0.49
2:U:147:LEU:HD11	2:U:197:TRP:CD1	2.47	0.49
2:U:147:LEU:HD13	2:U:219:ILE:HG21	1.94	0.49
1:R:9:LEU:HD21	1:R:66:TYR:HB3	1.92	0.49
2:J:38:LYS:HG3	2:J:94:TYR:HE1	1.77	0.49
2:U:164:ASN:HB2	2:U:202:VAL:HG13	1.93	0.49
1:D:19:ARG:HH11	1:D:157:ASP:HA	1.77	0.49
2:J:2:VAL:HG21	2:J:111:TYR:CD2	2.46	0.49
2:X:2:VAL:HG21	2:X:111:TYR:CD2	2.47	0.49
2:H:61:ASN:OD1	2:H:62:GLN:N	2.45	0.49
1:R:220:LEU:HG	1:R:263:ILE:HD12	1.94	0.49
1:A:85:ILE:HD11	1:A:112:ILE:HD11	1.95	0.49
1:C:9:LEU:HD21	1:C:66:TYR:HB3	1.95	0.49
2:V:2:VAL:HG21	2:V:111:TYR:CD2	2.48	0.49
3:O:118:VAL:HG13	3:O:207:LYS:HD3	1.95	0.49
1:A:39:ILE:HB	1:A:178:LEU:HD11	1.94	0.49
3:Z:123:PRO:HB3	3:Z:134:THR:H	1.77	0.49
3:L:37:TRP:CE2	3:L:75:LEU:HB2	2.47	0.49
1:S:39:ILE:HB	1:S:178:LEU:HD11	1.92	0.49
6:T:403:FLC:OHB	6:T:403:FLC:OA1	2.20	0.49
3:K:120:LEU:HG	3:K:209:LEU:HD12	1.94	0.49
1:E:194:VAL:HG22	1:E:199:ILE:HG23	1.95	0.49
1:P:273:ILE:HG12	1:Q:215:PHE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:207:ILE:HD12	1:T:209:LEU:HD21	1.93	0.49
2:W:2:VAL:HG21	2:W:111:TYR:CD2	2.47	0.49
1:A:37:ARG:NH1	1:E:93:PRO:O	2.46	0.49
1:Q:230:VAL:O	1:Q:233:VAL:HG22	2.13	0.49
2:J:197:TRP:CH2	2:J:221:PRO:HB3	2.48	0.49
1:A:27:PRO:HG2	3:L:32:ILE:HD12	1.94	0.49
1:C:267:LEU:HD13	1:C:274:LYS:HE3	1.94	0.49
1:B:36:LEU:HD23	1:B:39:ILE:HD11	1.94	0.49
1:S:186:THR:HG22	1:S:207:ILE:HG22	1.95	0.49
2:X:61:ASN:OD1	2:X:62:GLN:N	2.45	0.49
1:T:224:SER:HB2	1:T:279:TRP:CZ3	2.47	0.49
2:H:60:TYR:HE1	2:H:70:LEU:HG	1.77	0.49
1:Q:254:LEU:HD12	1:R:251:THR:HG23	1.93	0.49
1:S:274:LYS:HZ2	1:T:215:PHE:HE1	1.59	0.49
3:O:36:ASN:HD21	2:I:108:TYR:HA	1.77	0.49
1:B:94:ASN:HD21	1:B:146:ILE:HA	1.78	0.49
2:W:174:THR:HG23	2:W:188:SER:HB2	1.95	0.49
1:Q:219:GLN:HB3	1:Q:220:LEU:HD12	1.94	0.49
1:C:197:THR:HG1	1:C:200:TYR:HE2	1.60	0.49
1:E:154:THR:HG23	1:E:156:LYS:H	1.78	0.48
1:D:219:GLN:HB3	1:D:220:LEU:HD12	1.95	0.48
3:N:122:PRO:HB3	3:N:209:LEU:HD21	1.95	0.48
1:R:37:ARG:HE	1:R:123:ARG:HD3	1.79	0.48
1:C:85:ILE:HD11	1:C:112:ILE:HD11	1.95	0.48
1:C:39:ILE:HB	1:C:178:LEU:HD11	1.95	0.48
1:P:19:ARG:HH11	1:P:157:ASP:HA	1.78	0.48
2:J:177:ALA:HB2	2:J:186:LEU:HD23	1.94	0.48
1:C:249:GLY:HA3	1:C:291:LEU:HD13	1.95	0.48
2:V:6:GLN:N	2:V:114:GLN:HE22	2.09	0.48
3:N:169:LYS:HA	3:N:175:TYR:CD1	2.48	0.48
1:E:219:GLN:HB3	1:E:220:LEU:HD12	1.95	0.48
1:T:19:ARG:HH11	1:T:157:ASP:HA	1.78	0.48
1:P:224:SER:HB2	1:P:279:TRP:CZ3	2.49	0.48
2:Y:61:ASN:OD1	2:Y:62:GLN:N	2.47	0.48
2:W:130:VAL:HG22	2:W:151:VAL:HG22	1.95	0.48
3:Z:85:GLU:HG3	3:Z:107:THR:HA	1.95	0.48
2:Y:30:THR:HA	2:Y:53:PRO:HB2	1.94	0.48
2:Y:205:ASN:N	2:Y:205:ASN:HD22	2.10	0.48
3:L:118:VAL:HG11	3:L:198:VAL:HG21	1.95	0.48
2:H:2:VAL:HG21	2:H:111:TYR:CD2	2.48	0.48
1:C:34:MET:SD	1:C:205:THR:HG21	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:152:LYS:HB2	2:G:195:SER:HB3	30.65	0.48
1:A:168:LEU:HD23	1:A:186:THR:HB	1.95	0.48
1:Q:252:THR:HG22	1:Q:287:ILE:HD13	1.95	0.48
2:J:207:ALA:HA	2:J:214:LYS:HA	1.94	0.48
1:C:230:VAL:O	1:C:233:VAL:HG22	2.14	0.48
2:X:98:ARG:NH2	2:X:110:ASP:OD2	2.33	0.48
1:E:37:ARG:HH21	1:E:123:ARG:CZ	2.27	0.48
3:N:135:LEU:HB2	3:N:181:LEU:HB3	1.96	0.48
1:B:273:ILE:HG12	1:C:215:PHE:HA	1.96	0.48
2:H:147:LEU:HD13	2:H:219:ILE:HG21	1.95	0.48
2:H:147:LEU:HA	3:L:121:PHE:CZ	2.48	0.48
1:S:154:THR:OG1	1:S:155:THR:N	2.45	0.48
2:W:163:TRP:CZ3	2:W:204:CYS:HB3	2.49	0.48
2:W:132:PRO:HG3	2:W:217:LYS:HB3	1.94	0.48
2:H:50:LEU:CD2	2:H:59:SER:HB3	2.44	0.48
1:P:168:LEU:HD23	1:P:186:THR:HB	1.95	0.48
2:G:128:PRO:HB3	2:G:154:TYR:HB3	1.95	0.48
1:S:19:ARG:HG2	1:S:20:PRO:HD2	1.95	0.48
1:E:138:PRO:HD2	1:E:139:MET:HE3	1.94	0.48
2:X:6:GLN:H	2:X:114:GLN:NE2	2.10	0.48
1:A:249:GLY:HA3	1:A:291:LEU:HD13	1.96	0.48
1:D:95:GLU:HA	1:D:128:LEU:HD23	1.96	0.48
2:G:130:VAL:HG12	2:G:151:VAL:HG22	1.96	0.48
1:T:249:GLY:HA3	1:T:291:LEU:HD13	1.95	0.47
1:Q:34:MET:SD	1:Q:205:THR:HG21	2.53	0.47
2:G:2:VAL:HG21	2:G:111:TYR:CD2	2.50	0.47
2:G:61:ASN:OD1	2:G:62:GLN:N	2.47	0.47
1:D:224:SER:HB2	1:D:279:TRP:CZ3	2.49	0.47
2:W:164:ASN:HD21	2:W:202:VAL:HG12	1.79	0.47
1:R:219:GLN:HB3	1:R:220:LEU:HD12	1.95	0.47
2:U:156:PRO:HD2	2:U:210:ALA:HB1	1.95	0.47
1:D:138:PRO:HD2	1:D:139:MET:HE3	1.96	0.47
3:K:211:ARG:O	3:K:211:ARG:NH1	2.48	0.47
2:H:145:VAL:HG23	2:H:194:SER:HB3	1.97	0.47
2:U:164:ASN:HB3	2:U:167:SER:HB2	1.95	0.47
1:D:194:VAL:HG22	1:D:199:ILE:HG23	1.96	0.47
1:E:79:LEU:HD11	1:E:83:HIS:HB2	1.95	0.47
2:W:144:MET:HA	2:W:193:PRO:HA	1.96	0.47
1:S:138:PRO:HD2	1:S:139:MET:HE3	1.95	0.47
1:A:254:LEU:HD12	1:B:251:THR:HG23	1.95	0.47
2:Y:6:GLN:N	2:Y:114:GLN:HE22	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:6:GLN:N	2:J:114:GLN:HE22	2.11	0.47
1:E:220:LEU:HG	1:E:263:ILE:HD12	1.96	0.47
3:M:169:LYS:HA	3:M:175:TYR:HD1	1.78	0.47
1:S:170:LEU:HD23	1:S:174:LEU:HD22	1.95	0.47
2:X:30:THR:HA	2:X:53:PRO:HB2	1.96	0.47
1:D:137:TYR:H	1:D:275:ALA:HB3	1.79	0.47
2:G:6:GLN:N	2:G:114:GLN:HE22	2.12	0.47
1:E:9:LEU:HD21	1:E:66:TYR:HB3	1.97	0.47
1:Q:37:ARG:HH21	1:Q:123:ARG:CZ	2.28	0.47
1:B:137:TYR:O	1:B:275:ALA:HB3	2.15	0.47
1:A:192:THR:HG23	1:A:200:TYR:O	2.14	0.47
2:U:216:ASP:OD1	2:U:216:ASP:N	2.48	0.47
1:D:36:LEU:HD23	1:D:39:ILE:HD11	1.96	0.47
1:Q:224:SER:HB2	1:Q:279:TRP:CH2	2.50	0.47
2:F:133:LEU:HD11	2:F:150:LEU:HB2	1.96	0.47
1:S:194:VAL:HG22	1:S:199:ILE:HG23	1.96	0.47
3:Z:22:CYS:HB3	3:Z:73:ALA:HB3	1.96	0.47
1:T:213:PHE:HE2	1:T:217:LEU:HD22	1.80	0.47
1:R:250:VAL:HB	1:S:251:THR:HG21	1.97	0.47
2:F:6:GLN:N	2:F:114:GLN:HE22	2.07	0.47
3:L:30:THR:OG1	3:L:32:ILE:HG12	2.14	0.47
1:B:37:ARG:HH21	1:B:123:ARG:CZ	2.28	0.47
1:Q:154:THR:OG1	1:Q:155:THR:N	2.45	0.47
1:A:207:ILE:HD12	1:A:209:LEU:HD21	1.96	0.47
2:X:164:ASN:HB2	2:X:168:LEU:HD13	1.96	0.47
1:P:85:ILE:HD11	1:P:112:ILE:HD11	1.96	0.47
1:Q:79:LEU:HD11	1:Q:83:HIS:HB2	1.96	0.47
2:W:52:ASN:HB3	2:W:55:ASN:HB2	1.96	0.47
1:T:328:PHE:CE2	1:T:332:ILE:HD11	2.50	0.47
1:D:85:ILE:HD11	1:D:112:ILE:HD11	1.96	0.47
2:W:61:ASN:OD1	2:W:62:GLN:N	2.47	0.47
1:S:271:SER:O	1:T:212:GLU:HB2	2.15	0.47
1:B:27:PRO:HG2	3:N:32:ILE:HD12	1.96	0.47
3:M:197:GLN:HB3	3:M:206:GLU:HG2	1.97	0.47
2:F:155:PHE:HA	2:F:156:PRO:HA	1.72	0.47
2:V:208:HIS:CE1	2:V:210:ALA:HB3	2.49	0.47
1:A:215:PHE:HA	1:E:273:ILE:HG12	1.97	0.47
2:Y:121:SER:OG	2:Y:182:ASP:OD1	2.33	0.47
1:Q:138:PRO:HD2	1:Q:139:MET:CE	2.44	0.47
2:F:48:ILE:HG23	2:F:64:PHE:CD2	2.50	0.47
3:L:118:VAL:HG12	3:L:139:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:LEU:HG	1:C:263:ILE:HD12	1.96	0.47
1:C:154:THR:OG1	1:C:155:THR:N	2.47	0.47
2:U:30:THR:HA	2:U:53:PRO:HB2	1.97	0.47
1:Q:274:LYS:HZ2	1:R:215:PHE:HE1	1.62	0.46
1:C:137:TYR:H	1:C:275:ALA:HB3	1.79	0.46
3:N:120:LEU:HD12	3:N:209:LEU:HB2	1.97	0.46
3:O:22:CYS:HB3	3:O:73:ALA:HB3	1.98	0.46
2:I:6:GLN:H	2:I:114:GLN:NE2	2.12	0.46
2:F:38:LYS:HG3	2:F:94:TYR:HE1	1.80	0.46
1:S:252:THR:HG22	1:S:287:ILE:HD13	1.95	0.46
2:V:140:GLN:C	2:V:142:ASN:H	2.19	0.46
1:D:252:THR:HG22	1:D:287:ILE:HD13	1.96	0.46
1:B:267:LEU:HD13	1:B:274:LYS:HE3	1.97	0.46
1:Q:194:VAL:HG22	1:Q:199:ILE:HG23	1.96	0.46
1:P:79:LEU:HD11	1:P:83:HIS:HB2	1.98	0.46
2:I:2:VAL:HG21	2:I:111:TYR:CD2	2.50	0.46
2:H:197:TRP:CD1	2:H:198:PRO:HA	2.50	0.46
2:F:152:LYS:HZ2	3:N:134:THR:HG1	1.58	0.46
1:S:79:LEU:HD11	1:S:83:HIS:HB2	1.97	0.46
1:B:230:VAL:O	1:B:233:VAL:HG22	2.15	0.46
1:A:274:LYS:NZ	1:B:215:PHE:HE1	2.13	0.46
1:A:279:TRP:HB2	1:A:334:TYR:CZ	2.51	0.46
2:F:98:ARG:NH2	2:F:110:ASP:OD2	2.35	0.46
1:Q:94:ASN:OD1	1:Q:94:ASN:N	2.40	0.46
3:L:159:THR:OG1	3:L:160:GLN:N	2.48	0.46
1:E:95:GLU:OE2	1:E:100:LYS:NZ	2.46	0.46
2:J:61:ASN:OD1	2:J:62:GLN:N	2.48	0.46
1:P:220:LEU:HG	1:P:263:ILE:HD12	1.98	0.46
3:Z:170:GLN:HG2	3:Z:174:LYS:O	2.15	0.46
2:H:30:THR:HA	2:H:53:PRO:HB2	1.97	0.46
1:R:154:THR:HG23	1:R:156:LYS:H	1.81	0.46
1:D:137:TYR:O	1:D:275:ALA:HB3	2.16	0.46
2:V:13:ARG:NH2	2:V:124:LYS:HD2	2.30	0.46
1:Q:154:THR:HG23	1:Q:156:LYS:H	1.81	0.46
1:B:224:SER:HB2	1:B:279:TRP:CZ3	2.51	0.46
2:V:98:ARG:NH2	2:V:110:ASP:OD2	2.36	0.46
2:V:213:THR:HG22	2:V:215:VAL:HG23	1.98	0.46
2:U:168:LEU:HG	2:U:170:SER:H	1.80	0.46
3:K:123:PRO:HD3	3:K:135:LEU:HG	1.98	0.46
1:A:94:ASN:N	1:A:94:ASN:OD1	2.42	0.46
2:Y:143:SER:OG	2:Y:144:MET:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:O	1:A:233:VAL:HG22	2.16	0.46
3:K:132:LYS:HA	3:K:184:THR:HA	1.98	0.46
2:U:38:LYS:HG3	2:U:94:TYR:HE1	1.81	0.46
3:M:119:THR:HA	3:M:207:LYS:HE2	1.97	0.46
2:V:172:VAL:HG22	2:V:190:VAL:HB	1.97	0.46
5:B:402:LMT:H6D	5:B:402:LMT:H3B	1.96	0.46
3:Z:152:LYS:HG3	3:Z:157:PRO:HD3	1.99	0.45
1:R:249:GLY:HA3	1:R:291:LEU:HD13	1.98	0.45
1:E:230:VAL:O	1:E:233:VAL:HG22	2.16	0.45
1:A:219:GLN:HB3	1:A:220:LEU:HD12	1.97	0.45
3:N:152:LYS:HB2	3:N:195:SER:HB2	1.96	0.45
1:Q:228:VAL:O	1:Q:231:SER:OG	2.27	0.45
3:N:115:SER:HA	3:N:116:PRO:HD3	1.84	0.45
1:R:207:ILE:HD12	1:R:209:LEU:HD21	1.97	0.45
1:A:319:SER:HA	1:A:322:LEU:HB3	1.98	0.45
2:V:181:SER:OG	2:V:182:ASP:N	2.48	0.45
3:O:137:CYS:HB2	3:O:151:TRP:CH2	2.51	0.45
3:K:91:ALA:HB2	3:K:100:PHE:CD2	2.50	0.45
1:S:96:LYS:O	1:S:127:VAL:HB	2.16	0.45
1:E:33:ASN:OD1	1:E:56:ARG:NH1	2.48	0.45
3:M:30:THR:OG1	3:M:32:ILE:HG12	2.17	0.45
2:Y:155:PHE:HB2	2:Y:183:LEU:HD23	1.99	0.45
1:S:254:LEU:HD12	1:T:251:THR:HG23	1.98	0.45
3:K:37:TRP:CD2	3:K:75:LEU:HB2	2.51	0.45
2:V:60:TYR:HE1	2:V:70:LEU:HG	1.80	0.45
1:D:230:VAL:O	1:D:233:VAL:HG22	2.16	0.45
3:O:107:THR:HG21	3:O:144:PRO:HB3	1.98	0.45
3:K:128:LEU:HD11	3:K:188:TRP:HZ3	1.81	0.45
1:A:252:THR:HG22	1:A:287:ILE:HD13	1.97	0.45
1:R:308:TRP:CE3	1:R:311:ILE:HD12	2.52	0.45
1:C:94:ASN:OD1	1:C:94:ASN:N	2.47	0.45
1:T:138:PRO:HD2	1:T:139:MET:CE	2.46	0.45
1:B:19:ARG:HG2	1:B:20:PRO:HD2	1.99	0.45
2:U:2:VAL:HG21	2:U:111:TYR:CD2	2.51	0.45
1:E:170:LEU:O	2:I:54:TYR:OH	2.32	0.45
2:W:60:TYR:HE1	2:W:70:LEU:HG	1.82	0.45
1:B:85:ILE:HD11	1:B:112:ILE:HD11	1.99	0.45
3:L:151:TRP:CZ3	3:L:196:CYS:HB2	2.52	0.45
1:E:194:VAL:O	2:J:55:ASN:ND2	2.49	0.45
1:T:194:VAL:HB	2:Y:52:ASN:HD22	1.82	0.45
1:S:19:ARG:HH11	1:S:157:ASP:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:20:PRO:HD3	1:S:86:TRP:CD2	2.51	0.45
1:D:267:LEU:HD13	1:D:274:LYS:HE3	1.99	0.45
3:K:188:TRP:HD1	3:K:194:TYR:OH	2.00	0.45
1:B:138:PRO:HD2	1:B:139:MET:HE3	1.99	0.45
1:E:19:ARG:HH11	1:E:157:ASP:HA	1.82	0.45
2:W:144:MET:HG2	2:W:193:PRO:HA	1.99	0.44
1:S:230:VAL:O	1:S:233:VAL:HG22	2.16	0.44
1:C:224:SER:HB2	1:C:279:TRP:CZ3	2.51	0.44
1:D:168:LEU:HD23	1:D:186:THR:HB	1.99	0.44
1:Q:137:TYR:O	1:Q:275:ALA:HB3	2.17	0.44
2:H:60:TYR:CE1	2:H:70:LEU:HG	2.52	0.44
2:I:197:TRP:CD2	2:I:198:PRO:HA	2.52	0.44
3:O:159:THR:OG1	3:O:160:GLN:N	2.50	0.44
1:S:273:ILE:HG12	1:T:215:PHE:HA	1.99	0.44
2:U:61:ASN:OD1	2:U:62:GLN:N	2.50	0.44
1:T:95:GLU:HA	1:T:128:LEU:HD23	1.99	0.44
1:D:20:PRO:HA	1:D:21:PRO:HD3	1.81	0.44
2:U:155:PHE:HA	2:U:156:PRO:HA	1.79	0.44
1:B:137:TYR:H	1:B:275:ALA:HB3	1.82	0.44
2:J:51:ILE:HB	2:J:58:THR:HG22	1.99	0.44
2:W:50:LEU:CD2	2:W:59:SER:HB3	2.47	0.44
3:L:152:LYS:HB2	3:L:195:SER:HB3	1.98	0.44
1:S:217:LEU:HD12	1:S:221:TYR:HB2	1.99	0.44
1:A:26:GLY:HA2	3:L:95:SER:OG	2.18	0.44
1:D:37:ARG:HE	1:D:123:ARG:HD3	1.83	0.44
1:S:207:ILE:HD12	1:S:209:LEU:HD21	1.99	0.44
2:X:168:LEU:HD23	2:X:190:VAL:HG21	1.99	0.44
1:P:9:LEU:HD21	1:P:66:TYR:HB3	2.00	0.44
1:P:96:LYS:O	1:P:127:VAL:HB	2.18	0.44
1:E:96:LYS:O	1:E:127:VAL:HB	2.18	0.44
1:P:36:LEU:HD23	1:P:39:ILE:HD11	1.99	0.44
1:T:154:THR:HG23	1:T:156:LYS:H	1.83	0.44
3:L:68:LEU:HD23	3:L:73:ALA:HA	1.99	0.44
1:Q:37:ARG:HE	1:Q:123:ARG:HD3	1.82	0.44
1:A:9:LEU:HD21	1:A:66:TYR:HB3	2.00	0.44
2:X:38:LYS:HG3	2:X:94:TYR:HE1	1.82	0.44
1:Q:139:MET:HG2	1:Q:139:MET:H	1.64	0.44
2:I:14:PRO:HG2	2:I:122:SER:HB3	1.98	0.44
1:B:217:LEU:O	1:B:222:ILE:HG12	2.17	0.44
2:W:140:GLN:HG3	2:W:145:VAL:HG23	1.99	0.44
1:B:219:GLN:HB3	1:B:220:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ARG:HG2	1:D:20:PRO:HD2	2.00	0.44
1:P:217:LEU:O	1:P:222:ILE:HG12	2.17	0.44
1:C:250:VAL:HG21	1:D:247:THR:HG22	2.00	0.44
1:R:194:VAL:HG23	2:V:105:TYR:HB2	1.99	0.44
1:D:181:PHE:HB3	1:D:209:LEU:HB3	2.00	0.44
1:A:215:PHE:HE1	1:E:274:LYS:NZ	2.15	0.44
1:P:219:GLN:HB3	1:P:220:LEU:HD12	2.00	0.44
1:P:137:TYR:HA	1:P:138:PRO:HA	1.77	0.44
1:P:138:PRO:HD2	1:P:139:MET:HE3	1.99	0.44
3:O:41:LYS:HB2	3:O:45:LEU:HB2	2.00	0.44
1:S:37:ARG:HH21	1:S:123:ARG:CZ	2.31	0.44
1:S:85:ILE:HD11	1:S:112:ILE:HD11	2.00	0.43
3:L:135:LEU:HB2	3:L:181:LEU:HB3	2.00	0.43
3:L:154:ASP:OD2	3:L:191:HIS:ND1	2.36	0.43
1:E:137:TYR:CB	1:E:274:LYS:HB3	2.48	0.43
2:V:60:TYR:CE1	2:V:70:LEU:HG	2.54	0.43
3:O:85:GLU:HG3	3:O:107:THR:HA	1.99	0.43
1:R:185:ASN:OD1	4:R:401:NAG:N2	2.50	0.43
1:E:239:ARG:HD2	1:E:301:ALA:HB1	2.00	0.43
1:R:224:SER:HB2	1:R:279:TRP:CH2	2.54	0.43
1:R:232:TRP:CH2	1:R:324:PRO:HA	2.53	0.43
1:E:224:SER:HB2	1:E:279:TRP:CZ3	2.53	0.43
1:P:319:SER:HA	1:P:322:LEU:HB3	2.00	0.43
2:F:33:THR:HA	2:F:53:PRO:HD3	2.01	0.43
2:H:154:TYR:OH	2:H:186:LEU:HD23	2.19	0.43
1:A:33:ASN:HB3	1:A:56:ARG:HB2	1.99	0.43
1:T:36:LEU:HD23	1:T:39:ILE:HD11	2.00	0.43
2:W:30:THR:HA	2:W:53:PRO:HB2	2.00	0.43
1:B:319:SER:HA	1:B:322:LEU:HB3	1.99	0.43
3:L:111:GLN:NE2	3:L:172:ASN:O	2.49	0.43
2:H:155:PHE:HA	2:H:156:PRO:HA	1.84	0.43
2:F:146:THR:HB	3:N:119:THR:HG21	2.00	0.43
2:H:179:LEU:HD13	2:H:184:TYR:CD1	2.53	0.43
1:C:31:SER:HB2	1:C:58:SER:HB3	2.00	0.43
1:R:100:LYS:HA	1:R:100:LYS:HD3	1.78	0.43
1:Q:20:PRO:HD3	1:Q:86:TRP:CD2	2.54	0.43
3:N:127:GLU:O	3:N:130:THR:OG1	2.27	0.43
2:H:110:ASP:HB3	2:H:111:TYR:H	1.68	0.43
1:A:215:PHE:HE1	1:E:274:LYS:HZ2	1.64	0.43
2:F:2:VAL:HG21	2:F:111:TYR:CD2	2.53	0.43
2:G:45:LEU:O	3:K:100:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:O	1:A:127:VAL:HB	2.18	0.43
2:W:29:PHE:CD2	2:W:77:SER:HA	2.54	0.43
1:A:37:ARG:HE	1:A:123:ARG:HD3	1.83	0.43
2:G:202:VAL:O	2:G:218:LYS:HA	2.19	0.43
3:O:141:ASP:HA	3:O:174:LYS:HB3	2.01	0.43
1:S:250:VAL:HB	1:T:251:THR:HG21	1.99	0.43
1:D:273:ILE:HG12	1:E:215:PHE:HA	2.01	0.43
1:A:224:SER:HB2	1:A:279:TRP:CZ3	2.54	0.43
1:S:328:PHE:CE2	1:S:332:ILE:HD11	2.54	0.43
2:F:50:LEU:CD2	2:F:59:SER:HB3	2.49	0.43
3:K:77:ILE:HD11	3:K:88:TYR:HE2	1.84	0.43
1:R:138:PRO:HD2	1:R:139:MET:HE3	2.01	0.43
1:D:174:LEU:CD2	1:D:183:LEU:HD13	2.48	0.43
3:L:107:THR:HG21	3:L:144:PRO:HB3	2.01	0.43
1:E:267:LEU:HD13	1:E:274:LYS:HE3	1.99	0.43
1:E:137:TYR:H	1:E:275:ALA:HB3	1.83	0.43
2:W:11:LEU:HD12	2:W:119:THR:O	2.18	0.43
1:P:34:MET:SD	1:P:205:THR:HG21	2.58	0.43
1:D:217:LEU:O	1:D:222:ILE:HG12	2.18	0.43
1:Q:207:ILE:HD12	1:Q:209:LEU:HD21	2.01	0.43
2:H:193:PRO:O	2:H:196:THR:OG1	2.31	0.42
1:A:250:VAL:HB	1:B:251:THR:HG21	2.00	0.42
2:H:197:TRP:CG	2:H:198:PRO:HA	2.53	0.42
3:N:37:TRP:CZ3	3:N:90:CYS:HB3	2.54	0.42
1:D:154:THR:HG23	1:D:156:LYS:H	1.84	0.42
1:C:137:TYR:CB	1:C:274:LYS:HB3	2.49	0.42
1:P:66:TYR:CE2	1:P:114:ASN:HA	2.54	0.42
1:T:311:ILE:O	1:T:315:VAL:HG23	2.19	0.42
3:M:151:TRP:O	3:M:158:VAL:HB	2.19	0.42
1:R:137:TYR:O	1:R:275:ALA:HB3	2.19	0.42
1:D:317:LEU:HA	1:D:320:ARG:HD2	2.01	0.42
3:M:77:ILE:HD11	3:M:88:TYR:HE2	1.84	0.42
1:B:154:THR:HG23	1:B:156:LYS:H	1.84	0.42
2:F:152:LYS:NZ	3:N:134:THR:OG1	2.34	0.42
1:E:171:LYS:HG2	1:E:172:VAL:H	1.84	0.42
2:G:38:LYS:HG3	2:G:94:TYR:HE1	1.84	0.42
2:U:29:PHE:CD2	2:U:77:SER:HA	2.53	0.42
2:G:155:PHE:HA	2:G:156:PRO:HA	1.75	0.42
1:Q:49:TYR:CE1	1:Q:144:CYS:HB3	2.54	0.42
1:D:9:LEU:HD21	1:D:66:TYR:HB3	2.01	0.42
1:P:251:THR:HG23	1:T:254:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ARG:NE	1:C:123:ARG:HD3	2.32	0.42
2:W:208:HIS:NE2	2:W:210:ALA:HB3	2.34	0.42
3:K:151:TRP:CE3	3:K:181:LEU:HD22	2.55	0.42
1:P:19:ARG:HG2	1:P:20:PRO:HD2	2.01	0.42
1:D:279:TRP:HB2	1:D:334:TYR:CZ	2.55	0.42
1:E:161:LEU:HD11	3:M:32:ILE:HG22	2.00	0.42
3:N:77:ILE:HD11	3:N:88:TYR:HE2	1.84	0.42
1:Q:311:ILE:O	1:Q:315:VAL:HG23	2.19	0.42
2:W:38:LYS:HG3	2:W:94:TYR:HE1	1.84	0.42
2:Y:2:VAL:HG21	2:Y:111:TYR:CD2	2.54	0.42
2:G:60:TYR:CE1	2:G:70:LEU:HG	2.55	0.42
1:Q:226:MET:O	1:Q:230:VAL:HG23	2.19	0.42
1:E:259:GLN:O	1:E:263:ILE:HG12	2.20	0.42
1:D:137:TYR:CB	1:D:274:LYS:HB3	2.49	0.42
1:P:58:SER:HA	1:P:118:VAL:O	2.20	0.42
1:A:109:LEU:HB3	1:A:121:SER:HB3	2.02	0.42
1:E:181:PHE:HB3	1:E:209:LEU:HB3	1.99	0.42
1:R:20:PRO:HA	1:R:21:PRO:HD3	1.83	0.42
2:F:45:LEU:O	3:N:100:PHE:HB2	2.19	0.42
3:L:91:ALA:HB2	3:L:100:PHE:CD2	2.54	0.42
3:O:186:ARG:HD3	3:O:190:ARG:HH22	1.83	0.42
1:T:109:LEU:HB3	1:T:121:SER:HB3	2.00	0.42
1:R:254:LEU:HD12	1:S:251:THR:HG23	2.01	0.42
2:W:6:GLN:H	2:W:114:GLN:NE2	2.17	0.42
1:E:56:ARG:HA	1:E:120:TYR:O	2.20	0.42
1:S:20:PRO:HA	1:S:21:PRO:HD3	1.82	0.42
1:T:319:SER:HA	1:T:322:LEU:HB3	2.01	0.42
1:P:227:LEU:HD21	1:P:255:THR:HG22	2.01	0.42
3:Z:45:LEU:HA	3:Z:45:LEU:HD13	1.90	0.42
2:Y:60:TYR:HE1	2:Y:70:LEU:HG	1.84	0.42
1:P:154:THR:HG23	1:P:156:LYS:H	1.83	0.42
2:U:162:THR:O	2:U:204:CYS:HB2	2.20	0.42
1:B:325:VAL:O	1:B:329:VAL:HG23	2.20	0.42
1:P:37:ARG:HE	1:P:123:ARG:HD3	1.85	0.42
2:V:133:LEU:HB2	2:V:148:GLY:HA3	2.01	0.42
3:O:30:THR:OG1	3:O:32:ILE:HG12	2.19	0.42
2:G:11:LEU:HD12	2:G:119:THR:O	2.18	0.42
2:F:163:TRP:HZ2	2:F:188:SER:HB2	1.85	0.42
1:Q:33:ASN:HB3	1:Q:56:ARG:HB2	2.02	0.42
2:Y:163:TRP:CE2	2:Y:190:VAL:HB	2.54	0.42
1:S:137:TYR:O	1:S:275:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:250:VAL:HB	1:R:251:THR:HG21	2.02	0.42
3:N:37:TRP:CD2	3:N:75:LEU:HB2	2.54	0.42
2:H:143:SER:O	2:H:194:SER:OG	2.28	0.42
2:F:197:TRP:CD2	2:F:198:PRO:HD3	2.54	0.42
1:R:328:PHE:CE2	1:R:332:ILE:HD11	2.55	0.42
1:R:186:THR:HG22	1:R:207:ILE:HG22	2.01	0.42
3:O:37:TRP:CD2	3:O:75:LEU:HB2	2.54	0.42
1:S:267:LEU:HD13	1:S:274:LYS:HE3	2.02	0.42
1:R:259:GLN:O	1:R:263:ILE:HG12	2.20	0.42
2:I:29:PHE:CD2	2:I:77:SER:HA	2.55	0.42
3:O:60:VAL:HA	3:O:61:PRO:HD3	1.91	0.42
1:T:79:LEU:HD11	1:T:83:HIS:HB2	2.01	0.42
3:K:30:THR:OG1	3:K:32:ILE:HG12	2.20	0.42
1:D:22:THR:HG22	1:D:24:ASN:H	1.85	0.42
1:B:96:LYS:O	1:B:127:VAL:HB	2.19	0.42
3:O:164:THR:HG23	3:O:179:SER:HB2	2.01	0.42
2:F:11:LEU:HD12	2:F:119:THR:O	2.20	0.42
2:X:155:PHE:HA	2:X:156:PRO:HA	1.81	0.42
1:B:56:ARG:HA	1:B:120:TYR:O	2.19	0.42
1:A:217:LEU:O	1:A:222:ILE:HG12	2.19	0.42
1:D:56:ARG:HA	1:D:120:TYR:O	2.20	0.41
1:A:194:VAL:HG23	2:H:105:TYR:HB2	2.02	0.41
1:E:194:VAL:HG21	2:J:50:LEU:HD11	2.02	0.41
2:F:30:THR:HA	2:F:53:PRO:HB2	2.01	0.41
1:C:319:SER:HA	1:C:322:LEU:HB3	2.02	0.41
2:H:146:THR:HG22	2:H:191:THR:HB	2.01	0.41
1:E:94:ASN:HD21	1:E:146:ILE:HA	1.85	0.41
2:J:30:THR:O	2:J:54:TYR:HB2	2.20	0.41
1:D:95:GLU:OE2	1:D:100:LYS:NZ	2.52	0.41
1:A:181:PHE:HB3	1:A:209:LEU:HB3	2.03	0.41
1:Q:181:PHE:HB3	1:Q:209:LEU:HB3	2.01	0.41
3:Z:120:LEU:HG	3:Z:209:LEU:HD21	2.02	0.41
2:J:48:ILE:HG12	2:J:64:PHE:CE2	2.54	0.41
1:D:79:LEU:HD11	1:D:83:HIS:HB2	2.02	0.41
2:V:36:TRP:CZ3	2:V:96:CYS:HB3	2.55	0.41
1:R:213:PHE:HE2	1:R:217:LEU:HD22	1.86	0.41
1:B:111:ARG:HD2	1:B:119:LEU:HD23	2.00	0.41
1:B:181:PHE:HB3	1:B:209:LEU:HB3	2.03	0.41
2:H:6:GLN:N	2:H:114:GLN:HE22	2.16	0.41
2:W:208:HIS:HA	2:W:209:PRO:HD2	1.94	0.41
1:C:274:LYS:NZ	1:D:215:PHE:HE1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:60:TYR:HE1	2:G:70:LEU:HG	1.85	0.41
3:Z:41:LYS:HB2	3:Z:45:LEU:HB2	2.02	0.41
2:V:100:GLY:HA3	2:V:108:TYR:CZ	2.56	0.41
2:J:126:THR:HA	2:J:127:PRO:HD3	1.85	0.41
1:P:88:PRO:O	1:P:90:THR:N	2.52	0.41
3:N:137:CYS:HB3	3:N:179:SER:HB3	2.02	0.41
2:H:222:ARG:HA	2:H:222:ARG:HD2	1.87	0.41
1:P:100:LYS:HA	1:P:100:LYS:HD3	1.77	0.41
1:C:250:VAL:HB	1:D:251:THR:HG21	2.02	0.41
2:J:52:ASN:HB3	2:J:55:ASN:HB2	2.02	0.41
1:R:37:ARG:NE	1:R:123:ARG:HD3	2.35	0.41
3:L:118:VAL:HG12	3:L:139:ILE:HG23	2.02	0.41
1:Q:19:ARG:HH11	1:Q:157:ASP:HA	1.86	0.41
2:V:108:TYR:HA	3:Z:36:ASN:HD21	1.84	0.41
2:H:132:PRO:O	3:L:124:SER:HB3	2.20	0.41
2:U:133:LEU:HD11	2:U:150:LEU:HB2	2.02	0.41
2:V:30:THR:HA	2:V:53:PRO:HB2	2.02	0.41
1:D:321:ALA:C	1:D:324:PRO:HD2	2.40	0.41
3:O:71:ASP:N	3:O:71:ASP:OD1	2.53	0.41
1:A:100:LYS:HA	1:A:100:LYS:HD3	1.79	0.41
1:C:194:VAL:HG13	1:C:199:ILE:HG12	2.02	0.41
1:R:170:LEU:O	2:U:54:TYR:OH	2.34	0.41
1:C:181:PHE:HB3	1:C:209:LEU:HB3	2.03	0.41
1:R:181:PHE:HB3	1:R:209:LEU:HB3	2.03	0.41
1:C:219:GLN:HB3	1:C:220:LEU:HD12	2.01	0.41
1:Q:19:ARG:HG2	1:Q:20:PRO:HD2	2.02	0.41
1:T:130:CYS:HA	1:T:131:PRO:HD2	1.91	0.41
1:D:130:CYS:HA	1:D:131:PRO:HD2	1.89	0.41
1:R:95:GLU:HA	1:R:128:LEU:HD23	2.02	0.41
2:F:163:TRP:CZ2	2:F:188:SER:HB2	2.56	0.41
1:T:219:GLN:HB3	1:T:220:LEU:HD12	2.02	0.41
1:S:219:GLN:HB3	1:S:220:LEU:HD12	2.02	0.41
1:D:85:ILE:O	1:D:87:MET:HG3	2.20	0.41
1:T:95:GLU:OE2	1:T:100:LYS:NZ	2.51	0.41
1:C:217:LEU:O	1:C:222:ILE:HG12	2.21	0.41
3:K:41:LYS:HE2	3:K:83:GLU:O	2.21	0.41
1:P:135:GLN:OE1	1:P:135:GLN:N	2.53	0.41
2:W:6:GLN:N	2:W:114:GLN:HE22	2.15	0.41
1:T:37:ARG:NE	1:T:123:ARG:HD3	2.36	0.41
1:S:274:LYS:HE2	1:S:274:LYS:HB2	1.90	0.41
1:B:137:TYR:CB	1:B:274:LYS:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:321:ALA:C	1:T:324:PRO:HD2	2.41	0.41
2:F:175:PHE:HA	2:F:176:PRO:HD3	1.87	0.41
3:L:186:ARG:O	3:L:190:ARG:HB2	2.21	0.41
1:R:242:ILE:HG21	1:S:244:ALA:HB2	2.03	0.41
1:A:250:VAL:HG21	1:B:247:THR:HG22	2.02	0.41
1:D:33:ASN:HB3	1:D:56:ARG:HB2	2.03	0.41
3:Z:37:TRP:CD2	3:Z:75:LEU:HB2	2.55	0.41
1:D:137:TYR:HB3	1:D:274:LYS:HB3	2.03	0.41
3:O:68:LEU:HD23	3:O:73:ALA:HA	2.03	0.41
1:A:137:TYR:CB	1:A:274:LYS:HB3	2.51	0.41
1:A:19:ARG:HH11	1:A:157:ASP:HA	1.86	0.41
2:G:50:LEU:CD2	2:G:59:SER:HB3	2.51	0.41
2:W:219:ILE:HD13	2:W:219:ILE:HA	1.91	0.41
3:N:120:LEU:HD22	3:N:121:PHE:H	1.85	0.41
2:J:177:ALA:HA	2:J:186:LEU:HB3	2.03	0.41
1:S:137:TYR:H	1:S:275:ALA:HB3	1.86	0.41
1:S:137:TYR:HA	1:S:138:PRO:HA	1.77	0.41
1:E:137:TYR:O	1:E:275:ALA:HB3	2.20	0.41
2:I:198:PRO:HB3	2:I:221:PRO:HG3	2.02	0.41
1:Q:20:PRO:HA	1:Q:21:PRO:HD3	1.82	0.41
2:W:27:TYR:CE2	2:W:29:PHE:HA	2.56	0.41
1:P:37:ARG:HH21	1:P:123:ARG:CZ	2.33	0.41
1:R:274:LYS:NZ	1:S:215:PHE:HE1	2.18	0.41
2:F:47:TRP:CH2	2:F:49:GLY:HA2	2.55	0.41
2:H:162:THR:OG1	2:H:205:ASN:HB2	2.21	0.41
2:W:155:PHE:HA	2:W:156:PRO:HA	1.81	0.41
2:I:48:ILE:HG12	2:I:64:PHE:CE2	2.56	0.41
1:Q:109:LEU:HB3	1:Q:121:SER:HB3	2.02	0.41
2:W:205:ASN:ND2	2:W:216:ASP:OD2	2.53	0.41
3:M:41:LYS:HE2	3:M:83:GLU:O	2.21	0.41
3:N:170:GLN:HG2	3:N:171:SER:H	1.85	0.41
1:T:275:ALA:HB1	1:T:338:PHE:CD2	2.55	0.41
1:P:33:ASN:HB3	1:P:56:ARG:HB2	2.02	0.41
2:V:124:LYS:HB3	2:V:124:LYS:HE3	1.89	0.41
1:D:27:PRO:HG2	3:O:32:ILE:HD12	2.03	0.41
1:R:162:TRP:CE2	1:R:203:LEU:HB3	2.56	0.41
3:M:159:THR:OG1	3:M:160:GLN:N	2.54	0.41
1:C:317:LEU:HA	1:C:320:ARG:HD2	2.03	0.41
2:H:48:ILE:HG23	2:H:64:PHE:CD2	2.56	0.41
1:C:20:PRO:HA	1:C:21:PRO:HD3	1.82	0.41
2:J:179:LEU:HD22	2:J:184:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:160:THR:OG1	2:H:207:ALA:HB3	2.21	0.40
1:T:217:LEU:HD12	1:T:221:TYR:HB2	2.03	0.40
1:E:94:ASN:N	1:E:94:ASN:OD1	2.45	0.40
1:P:207:ILE:HD12	1:P:209:LEU:HD21	2.03	0.40
2:V:149:CYS:HB2	2:V:163:TRP:CZ2	2.56	0.40
1:A:139:MET:HG2	1:A:139:MET:H	1.73	0.40
1:Q:95:GLU:OE2	1:Q:100:LYS:NZ	2.52	0.40
1:P:190:TYR:O	2:W:104:ARG:NH1	2.54	0.40
1:D:274:LYS:NZ	1:E:215:PHE:HE1	2.19	0.40
2:G:45:LEU:HD13	2:G:45:LEU:HA	4.41	0.40
1:C:19:ARG:HA	1:C:20:PRO:HD3	1.92	0.40
3:Z:60:VAL:HA	3:Z:61:PRO:HD3	1.95	0.40
1:C:100:LYS:HA	1:C:100:LYS:HD3	1.81	0.40
1:E:33:ASN:HB3	1:E:56:ARG:HB2	2.02	0.40
1:Q:137:TYR:CB	1:Q:274:LYS:HB3	2.52	0.40
1:B:20:PRO:HD3	1:B:86:TRP:CD2	2.56	0.40
1:D:194:VAL:HG23	2:I:105:TYR:HB2	2.03	0.40
2:F:110:ASP:HB3	2:F:111:TYR:H	1.68	0.40
1:R:227:LEU:HD21	1:R:255:THR:HG22	2.03	0.40
1:S:211:ARG:HD3	1:S:216:TYR:CE2	2.56	0.40
3:L:121:PHE:HA	3:L:122:PRO:HD2	1.93	0.40
1:B:226:MET:O	1:B:230:VAL:HG23	2.21	0.40
2:X:163:TRP:HZ3	2:X:219:ILE:HD11	1.86	0.40
3:L:149:VAL:HG11	3:L:164:THR:HG21	2.03	0.40
1:E:31:SER:HB2	1:E:58:SER:HB3	2.03	0.40
2:I:127:PRO:HA	2:I:128:PRO:HD3	1.77	0.40
3:Z:135:LEU:HD13	3:Z:181:LEU:HD23	2.03	0.40
3:O:170:GLN:OE1	3:O:176:MET:HB3	2.22	0.40
1:S:34:MET:SD	1:S:205:THR:HG21	2.62	0.40
1:D:190:TYR:O	2:I:104:ARG:NH1	2.55	0.40
2:H:50:LEU:HD21	2:H:59:SER:HB3	2.03	0.40
1:D:100:LYS:HA	1:D:100:LYS:HD3	1.81	0.40
1:S:139:MET:HG2	1:S:139:MET:H	1.68	0.40
2:F:195:SER:C	2:F:198:PRO:HD2	2.42	0.40
1:S:232:TRP:CH2	1:S:324:PRO:HA	2.57	0.40
2:W:146:THR:HG22	2:W:191:THR:HB	2.02	0.40
1:P:46:ASN:ND2	1:Q:41:LYS:HE2	2.37	0.40
1:Q:319:SER:HA	1:Q:322:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

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	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	46	83
1	B	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	46	83
1	C	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	46	83
1	D	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	46	83
1	E	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	46	83
1	P	333/347 (96%)	320 (96%)	12 (4%)	1 (0%)	46	83
1	Q	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	46	83
1	R	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	46	83
1	S	333/347 (96%)	320 (96%)	12 (4%)	1 (0%)	46	83
1	T	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	46	83
2	F	220/224 (98%)	204 (93%)	16 (7%)	0	100	100
2	G	222/224 (99%)	197 (89%)	25 (11%)	0	100	100
2	H	221/224 (99%)	198 (90%)	23 (10%)	0	100	100
2	I	220/224 (98%)	204 (93%)	16 (7%)	0	100	100
2	J	221/224 (99%)	200 (90%)	21 (10%)	0	100	100
2	U	219/224 (98%)	195 (89%)	24 (11%)	0	100	100
2	V	222/224 (99%)	196 (88%)	25 (11%)	1 (0%)	34	77
2	W	222/224 (99%)	199 (90%)	23 (10%)	0	100	100
2	X	222/224 (99%)	201 (90%)	21 (10%)	0	100	100
2	Y	219/224 (98%)	192 (88%)	27 (12%)	0	100	100
3	K	210/215 (98%)	190 (90%)	20 (10%)	0	100	100
3	L	209/215 (97%)	195 (93%)	13 (6%)	1 (0%)	34	77
3	M	209/215 (97%)	190 (91%)	19 (9%)	0	100	100
3	N	209/215 (97%)	193 (92%)	15 (7%)	1 (0%)	34	77
3	O	209/215 (97%)	198 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	Z	213/215 (99%)	192 (90%)	20 (9%)	1 (0%)	34 77
3	f	212/215 (99%)	198 (93%)	14 (7%)	0	100 100
3	g	209/215 (97%)	185 (88%)	24 (12%)	0	100 100
3	h	209/215 (97%)	191 (91%)	18 (9%)	0	100 100
3	i	212/215 (99%)	192 (91%)	20 (9%)	0	100 100
All	All	7639/7860 (97%)	7122 (93%)	503 (7%)	14 (0%)	52 87

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	B	68	VAL
1	C	68	VAL
1	D	68	VAL
1	E	68	VAL
1	P	68	VAL
1	Q	68	VAL
1	R	68	VAL
1	S	68	VAL
1	T	68	VAL
2	V	172	VAL
3	Z	152	LYS
3	L	95	SER
3	N	167	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	305/316 (96%)	305 (100%)	0	100 100
1	B	305/316 (96%)	305 (100%)	0	100 100
1	C	305/316 (96%)	305 (100%)	0	100 100
1	D	305/316 (96%)	305 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	305/316 (96%)	305 (100%)	0	100 100
1	P	305/316 (96%)	305 (100%)	0	100 100
1	Q	305/316 (96%)	305 (100%)	0	100 100
1	R	305/316 (96%)	305 (100%)	0	100 100
1	S	305/316 (96%)	305 (100%)	0	100 100
1	T	305/316 (96%)	305 (100%)	0	100 100
2	F	191/193 (99%)	191 (100%)	0	100 100
2	G	193/193 (100%)	193 (100%)	0	100 100
2	H	192/193 (100%)	190 (99%)	2 (1%)	82 93
2	I	191/193 (99%)	191 (100%)	0	100 100
2	J	192/193 (100%)	192 (100%)	0	100 100
2	U	190/193 (98%)	190 (100%)	0	100 100
2	V	193/193 (100%)	192 (100%)	1 (0%)	92 97
2	W	193/193 (100%)	193 (100%)	0	100 100
2	X	193/193 (100%)	191 (99%)	2 (1%)	82 93
2	Y	190/193 (98%)	189 (100%)	1 (0%)	92 97
3	K	179/182 (98%)	178 (99%)	1 (1%)	90 97
3	L	179/182 (98%)	177 (99%)	2 (1%)	80 92
3	M	179/182 (98%)	178 (99%)	1 (1%)	90 97
3	N	179/182 (98%)	179 (100%)	0	100 100
3	O	179/182 (98%)	179 (100%)	0	100 100
3	Z	182/182 (100%)	182 (100%)	0	100 100
3	f	181/182 (100%)	180 (99%)	1 (1%)	90 97
3	g	179/182 (98%)	179 (100%)	0	100 100
3	h	179/182 (98%)	179 (100%)	0	100 100
3	i	181/182 (100%)	181 (100%)	0	100 100
All	All	6765/6910 (98%)	6754 (100%)	11 (0%)	95 99

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	52	ASN
2	H	149	CYS

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Mol	Chain	Res	Type
3	K	119	THR
3	L	71	ASP
3	L	130	THR
2	V	186	LEU
2	X	159	VAL
2	X	183	LEU
2	Y	205	ASN
3	f	130	THR
3	M	130	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	55	ASN
2	H	52	ASN
3	L	170	GLN
2	Y	55	ASN
2	Y	205	ASN
3	Z	96	ASN
3	f	96	ASN
3	g	172	ASN
3	g	197	GLN
3	h	96	ASN
3	i	96	ASN
2	J	55	ASN
3	M	96	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	401	1	14,14,15	0.25	0	15,19,21	0.53	0
5	LMT	A	402	-	24,24,36	1.17	2 (8%)	35,35,47	1.27	3 (8%)
6	FLC	A	403	-	3,12,12	0.71	0	3,17,17	0.78	0
4	NAG	B	401	1	14,14,15	0.68	0	15,19,21	0.78	0
5	LMT	B	402	-	24,24,36	1.21	2 (8%)	35,35,47	1.27	5 (14%)
4	NAG	C	401	1	14,14,15	0.56	0	15,19,21	2.02	4 (26%)
5	LMT	C	402	-	24,24,36	1.13	2 (8%)	35,35,47	1.32	6 (17%)
4	NAG	D	401	1	14,14,15	0.45	0	15,19,21	1.10	1 (6%)
5	LMT	D	402	-	24,24,36	1.11	2 (8%)	35,35,47	1.13	3 (8%)
4	NAG	E	401	1	14,14,15	0.31	0	15,19,21	0.57	0
5	LMT	E	402	-	24,24,36	1.17	2 (8%)	35,35,47	1.13	2 (5%)
4	NAG	P	401	1	14,14,15	0.52	0	15,19,21	1.53	1 (6%)
5	LMT	P	402	-	24,24,36	1.14	2 (8%)	35,35,47	1.24	3 (8%)
4	NAG	Q	401	1	14,14,15	0.69	1 (7%)	15,19,21	0.78	0
5	LMT	Q	402	-	24,24,36	1.12	2 (8%)	35,35,47	1.49	6 (17%)
4	NAG	R	401	1	14,14,15	0.46	0	15,19,21	0.58	0
5	LMT	R	402	-	24,24,36	1.12	2 (8%)	35,35,47	1.03	1 (2%)
4	NAG	S	401	1	14,14,15	0.35	0	15,19,21	1.26	1 (6%)
5	LMT	S	402	-	24,24,36	1.13	2 (8%)	35,35,47	1.27	3 (8%)
4	NAG	T	401	1	14,14,15	0.34	0	15,19,21	0.71	0
5	LMT	T	402	-	26,26,36	1.13	2 (7%)	37,37,47	0.98	2 (5%)
6	FLC	T	403	-	3,12,12	0.87	0	3,17,17	1.81	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	LMT	A	402	-	-	0/8/48/61	0/2/2/2
6	FLC	A	403	-	-	0/6/16/16	0/0/0/0
4	NAG	B	401	1	-	0/6/23/26	0/1/1/1
5	LMT	B	402	-	-	0/8/48/61	0/2/2/2
4	NAG	C	401	1	-	0/6/23/26	0/1/1/1
5	LMT	C	402	-	-	0/8/48/61	0/2/2/2
4	NAG	D	401	1	-	0/6/23/26	0/1/1/1
5	LMT	D	402	-	-	0/8/48/61	0/2/2/2
4	NAG	E	401	1	-	0/6/23/26	0/1/1/1
5	LMT	E	402	-	-	0/8/48/61	0/2/2/2
4	NAG	P	401	1	-	0/6/23/26	0/1/1/1
5	LMT	P	402	-	-	0/8/48/61	0/2/2/2
4	NAG	Q	401	1	-	0/6/23/26	0/1/1/1
5	LMT	Q	402	-	-	0/8/48/61	0/2/2/2
4	NAG	R	401	1	-	0/6/23/26	0/1/1/1
5	LMT	R	402	-	-	0/8/48/61	0/2/2/2
4	NAG	S	401	1	-	0/6/23/26	0/1/1/1
5	LMT	S	402	-	-	0/8/48/61	0/2/2/2
4	NAG	T	401	1	-	0/6/23/26	0/1/1/1
5	LMT	T	402	-	-	0/11/51/61	0/2/2/2
6	FLC	T	403	-	-	0/6/16/16	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	401	NAG	C1-C2	2.03	1.55	1.52
5	C	402	LMT	O5'-C1'	2.58	1.47	1.43
5	T	402	LMT	O5'-C1'	2.67	1.48	1.41
5	R	402	LMT	O5B-C1B	2.75	1.48	1.41
5	D	402	LMT	O5B-C1B	2.76	1.48	1.41
5	Q	402	LMT	O5'-C1'	2.77	1.48	1.43
5	P	402	LMT	O5B-C1B	2.78	1.49	1.41
5	D	402	LMT	O5'-C1'	2.79	1.48	1.43
5	B	402	LMT	O5'-C1'	2.79	1.48	1.43
5	R	402	LMT	O5'-C1'	2.80	1.48	1.43
5	A	402	LMT	O5'-C1'	2.82	1.48	1.43
5	S	402	LMT	O5'-C1'	2.84	1.48	1.43
5	S	402	LMT	O5B-C1B	2.84	1.49	1.41
5	T	402	LMT	O5B-C1B	2.90	1.49	1.41
5	E	402	LMT	O5'-C1'	2.90	1.48	1.43
5	A	402	LMT	O5B-C1B	2.93	1.49	1.41
5	C	402	LMT	O5B-C1B	2.95	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	402	LMT	O5B-C1B	3.00	1.49	1.41
5	E	402	LMT	O5B-C1B	3.00	1.49	1.41
5	P	402	LMT	O5'-C1'	3.07	1.48	1.43
5	B	402	LMT	O5B-C1B	3.19	1.50	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	NAG	C2-N2-C7	-4.09	117.78	123.04
4	S	401	NAG	C1-O5-C5	-3.94	107.25	112.25
4	D	401	NAG	C1-O5-C5	-3.30	108.06	112.25
5	Q	402	LMT	C1B-O1B-C4'	-3.17	109.72	118.01
4	C	401	NAG	C4-C3-C2	-2.72	107.00	111.23
5	R	402	LMT	C1B-O1B-C4'	-2.71	110.92	118.01
5	E	402	LMT	C1B-O1B-C4'	-2.61	111.19	118.01
5	P	402	LMT	C1B-O1B-C4'	-2.54	111.36	118.01
5	T	402	LMT	C1B-O1B-C4'	-2.52	111.42	118.01
6	T	403	FLC	CB-CA-CAC	-2.38	111.14	114.96
5	D	402	LMT	C1B-O1B-C4'	-2.35	111.86	118.01
5	C	402	LMT	C1B-O1B-C4'	-2.27	112.07	118.01
5	B	402	LMT	C6B-C5B-C4B	-2.25	107.46	113.02
4	C	401	NAG	C6-C5-C4	-2.12	107.79	113.02
6	T	403	FLC	CB-CG-CGC	-2.02	111.73	114.96
5	Q	402	LMT	C1B-C2B-C3B	2.02	113.95	109.97
5	C	402	LMT	O5B-C1B-C2B	2.07	114.53	110.28
5	T	402	LMT	C2'-C3'-C4'	2.10	114.22	109.60
5	A	402	LMT	C1B-O5B-C5B	2.17	117.95	113.75
5	D	402	LMT	C1'-C2'-C3'	2.17	113.66	110.43
5	A	402	LMT	C3B-C4B-C5B	2.19	114.01	110.20
5	B	402	LMT	O5'-C5'-C4'	2.28	114.56	109.75
5	B	402	LMT	O5B-C1B-C2B	2.35	115.10	110.28
5	E	402	LMT	O5B-C1B-C2B	2.39	115.18	110.28
5	C	402	LMT	C1B-C2B-C3B	2.54	114.98	109.97
5	D	402	LMT	C2'-C3'-C4'	2.61	115.33	109.60
5	Q	402	LMT	O5B-C1B-C2B	2.67	115.76	110.28
5	C	402	LMT	C3'-C4'-C5'	2.78	117.13	110.84
5	C	402	LMT	C2'-C3'-C4'	2.82	115.79	109.60
5	S	402	LMT	O5B-C5B-C4B	2.87	115.07	109.68
5	S	402	LMT	C1'-C2'-C3'	3.10	115.05	110.43
5	Q	402	LMT	C3'-C4'-C5'	3.14	117.94	110.84
5	B	402	LMT	C1B-O5B-C5B	3.17	119.89	113.75
5	S	402	LMT	C2'-C3'-C4'	3.38	117.03	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	402	LMT	C1'-C2'-C3'	3.47	115.59	110.43
5	P	402	LMT	C1'-C2'-C3'	3.50	115.64	110.43
5	P	402	LMT	O5'-C1'-C2'	3.61	115.55	109.80
5	C	402	LMT	O5'-C5'-C4'	3.71	117.58	109.75
5	B	402	LMT	O5B-C5B-C4B	3.79	116.80	109.68
5	A	402	LMT	O5B-C5B-C4B	3.81	116.83	109.68
5	Q	402	LMT	C2'-C3'-C4'	4.03	118.45	109.60
4	C	401	NAG	C1-O5-C5	5.03	118.63	112.25
4	P	401	NAG	C1-O5-C5	5.40	119.10	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	LMT	1	0
4	R	401	NAG	1	0
6	T	403	FLC	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	337/347 (97%)	0.21	5 (1%) 76 64	91, 137, 216, 241	0
1	B	337/347 (97%)	0.22	14 (4%) 40 28	100, 143, 229, 269	0
1	C	337/347 (97%)	0.20	3 (0%) 85 75	94, 140, 228, 260	0
1	D	337/347 (97%)	0.15	9 (2%) 58 43	103, 144, 219, 255	0
1	E	337/347 (97%)	0.24	16 (4%) 35 25	99, 146, 221, 259	0
1	P	337/347 (97%)	0.17	6 (1%) 71 58	92, 110, 180, 204	0
1	Q	337/347 (97%)	0.27	8 (2%) 62 47	88, 110, 175, 199	0
1	R	337/347 (97%)	0.16	3 (0%) 85 75	87, 105, 166, 183	0
1	S	337/347 (97%)	0.30	7 (2%) 67 52	83, 101, 171, 193	0
1	T	337/347 (97%)	0.17	5 (1%) 76 64	84, 109, 173, 203	0
2	F	222/224 (99%)	0.11	7 (3%) 51 37	112, 139, 215, 248	0
2	G	224/224 (100%)	0.12	11 (4%) 33 23	103, 168, 199, 209	0
2	H	223/224 (99%)	0.05	1 (0%) 93 88	84, 121, 151, 224	0
2	I	222/224 (99%)	-0.01	6 (2%) 58 43	105, 133, 203, 223	0
2	J	223/224 (99%)	0.53	30 (13%) 4 4	115, 163, 263, 278	0
2	U	221/224 (98%)	0.45	25 (11%) 7 6	121, 172, 241, 253	0
2	V	224/224 (100%)	0.07	12 (5%) 29 20	114, 154, 185, 261	0
2	W	224/224 (100%)	0.11	6 (2%) 58 43	102, 126, 145, 207	0
2	X	224/224 (100%)	0.07	3 (1%) 79 66	98, 118, 137, 187	0
2	Y	221/224 (98%)	0.71	34 (15%) 3 2	139, 197, 278, 297	0
3	K	212/215 (98%)	0.05	6 (2%) 56 42	104, 133, 187, 198	0
3	L	211/215 (98%)	0.07	1 (0%) 91 86	81, 109, 162, 172	0
3	M	211/215 (98%)	0.49	22 (10%) 8 6	118, 151, 247, 254	0
3	N	211/215 (98%)	-0.07	5 (2%) 62 47	111, 150, 173, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	O	211/215 (98%)	-0.08	2 (0%) 85 75	104, 134, 153, 160	0
3	Z	215/215 (100%)	0.08	5 (2%) 64 48	112, 161, 190, 244	0
3	f	214/215 (99%)	0.05	5 (2%) 64 48	101, 124, 138, 174	0
3	g	211/215 (98%)	0.83	37 (17%) 2 2	150, 223, 274, 281	0
3	h	211/215 (98%)	0.18	13 (6%) 24 16	119, 178, 207, 217	0
3	i	214/215 (99%)	0.04	0 100 100	99, 119, 138, 169	0
All	All	7719/7860 (98%)	0.20	307 (3%) 42 29	81, 134, 233, 297	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	g	164	THR	11.4
3	g	178	SER	10.7
3	M	123	PRO	9.5
2	Y	161	VAL	9.4
2	U	188	SER	9.0
2	J	150	LEU	8.8
2	J	161	VAL	8.7
3	g	135	LEU	8.7
3	g	165	THR	8.3
2	Y	188	SER	7.9
3	M	135	LEU	7.5
2	U	187	SER	7.3
3	g	177	ALA	7.2
2	J	176	PRO	6.8
2	J	175	PHE	6.7
2	Y	160	THR	6.6
2	U	161	VAL	6.6
3	g	133	ALA	6.6
2	J	187	SER	6.5
2	Y	149	CYS	6.5
1	A	244	ALA	6.4
3	M	122	PRO	6.4
3	M	206	GLU	6.3
3	g	134	THR	6.3
2	J	151	VAL	6.3
2	J	147	LEU	6.2
2	Y	189	SER	6.1
3	g	136	VAL	6.1
1	B	244	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
3	g	183	LEU	6.0
2	J	152	LYS	5.9
2	J	134	ALA	5.9
2	G	150	LEU	5.8
3	M	136	VAL	5.7
2	Y	187	SER	5.6
2	J	149	CYS	5.5
3	g	123	PRO	5.5
3	M	118	VAL	5.4
3	g	163	GLU	5.3
1	S	107	ASN	5.3
2	Y	150	LEU	5.3
3	M	177	ALA	5.3
1	A	239	ARG	5.2
3	g	166	GLN	5.1
1	B	248	LEU	5.1
2	J	133	LEU	5.1
2	J	148	GLY	4.9
2	J	130	VAL	4.9
2	Y	140	GLN	4.8
2	U	159	VAL	4.8
2	U	142	ASN	4.8
3	h	135	LEU	4.8
2	Y	162	THR	4.7
2	J	139	ALA	4.7
3	g	182	THR	4.7
3	g	88	TYR	4.6
3	g	122	PRO	4.5
2	U	186	LEU	4.5
2	U	189	SER	4.5
2	J	186	LEU	4.5
2	I	130	VAL	4.5
2	Y	135	PRO	4.4
1	Q	6	LEU	4.4
1	S	2	ASP	4.4
3	g	84	ASP	4.4
3	M	134	THR	4.3
2	Y	174	THR	4.3
2	G	151	VAL	4.3
3	M	180	TYR	4.2
3	M	121	PHE	4.2
2	Y	134	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	U	192	VAL	4.2
2	Y	141	THR	4.1
3	h	136	VAL	4.1
1	S	6	LEU	4.1
1	E	244	ALA	4.0
2	Y	159	VAL	4.0
3	M	139	ILE	4.0
2	I	150	LEU	4.0
2	J	188	SER	4.0
1	D	247	THR	4.0
3	h	139	ILE	4.0
2	J	189	SER	3.9
3	g	89	PHE	3.9
2	J	219	ILE	3.8
3	h	138	THR	3.8
2	I	132	PRO	3.7
2	G	130	VAL	3.7
2	X	140	GLN	3.7
1	S	1	SER	3.7
2	J	177	ALA	3.7
1	A	242	ILE	3.7
2	Y	151	VAL	3.6
3	f	121	PHE	3.6
3	K	109	LEU	3.6
2	J	174	THR	3.6
1	T	6	LEU	3.5
1	D	68	VAL	3.5
2	Y	152	LYS	3.5
1	Q	1	SER	3.5
2	I	161	VAL	3.4
3	g	18	VAL	3.4
2	U	74	LYS	3.4
1	B	291	LEU	3.4
2	J	185	THR	3.4
1	D	291	LEU	3.4
1	T	2	ASP	3.4
2	U	152	LYS	3.3
1	E	220	LEU	3.3
2	U	185	THR	3.3
2	U	150	LEU	3.3
1	P	64	LEU	3.2
1	C	248	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	g	39	GLN	3.2
3	g	38	VAL	3.2
3	g	106	LEU	3.2
2	J	136	GLY	3.2
2	U	147	LEU	3.2
3	g	109	LEU	3.2
3	g	132	LYS	3.1
1	S	106	PRO	3.1
2	U	151	VAL	3.1
2	W	140	GLN	3.1
3	g	87	ILE	3.1
1	A	245	ARG	3.1
1	E	237	PHE	3.1
2	G	187	SER	3.1
3	M	157	PRO	3.1
3	M	109	LEU	3.1
2	Y	158	PRO	3.0
1	Q	2	ASP	3.0
2	V	150	LEU	3.0
2	Y	186	LEU	3.0
3	M	178	SER	3.0
2	F	133	LEU	3.0
2	V	188	SER	3.0
3	h	178	SER	3.0
2	V	147	LEU	3.0
1	P	2	ASP	3.0
1	Q	3	SER	3.0
2	J	159	VAL	3.0
2	F	150	LEU	3.0
3	Z	64	PHE	3.0
3	g	139	ILE	3.0
2	Y	202	VAL	3.0
1	T	107	ASN	2.9
1	D	2	ASP	2.9
3	K	136	VAL	2.9
3	g	179	SER	2.9
1	A	237	PHE	2.9
1	Q	10	PHE	2.9
2	V	139	ALA	2.9
2	W	150	LEU	2.9
2	U	149	CYS	2.9
1	B	250	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	M	181	LEU	2.9
2	H	223	ASP	2.8
3	g	91	ALA	2.8
2	W	147	LEU	2.8
3	g	92	LEU	2.8
1	R	107	ASN	2.8
1	D	243	PRO	2.8
1	E	248	LEU	2.8
2	V	133	LEU	2.8
2	J	178	VAL	2.8
1	B	249	GLY	2.8
3	N	182	THR	2.7
2	Y	48	ILE	2.7
2	J	135	PRO	2.7
3	N	50	ILE	2.7
2	Y	109	PHE	2.7
3	K	134	THR	2.7
2	G	147	LEU	2.7
3	h	151	TRP	2.7
1	B	247	THR	2.7
2	Y	18	MET	2.7
3	f	120	LEU	2.7
1	E	241	ALA	2.7
1	E	64	LEU	2.7
2	J	160	THR	2.7
2	U	215	VAL	2.6
2	Y	168	LEU	2.6
2	V	142	ASN	2.6
2	G	178	VAL	2.6
2	U	206	VAL	2.6
2	Y	97	ALA	2.6
2	U	141	THR	2.6
3	K	135	LEU	2.6
1	B	64	LEU	2.6
1	D	132	MET	2.6
2	U	191	THR	2.5
3	Z	120	LEU	2.5
2	U	175	PHE	2.5
2	W	105	TYR	2.5
3	M	138	THR	2.5
3	g	138	THR	2.5
1	C	55	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	V	218	LYS	2.5
3	Z	49	LEU	2.5
3	O	134	THR	2.5
3	f	136	VAL	2.5
2	Y	203	THR	2.5
2	Y	83	LEU	2.5
3	M	100	PHE	2.5
2	G	177	ALA	2.5
2	F	149	CYS	2.5
1	D	248	LEU	2.5
1	C	169	GLN	2.5
3	h	177	ALA	2.5
2	U	105	TYR	2.4
2	Y	43	LYS	2.4
3	h	195	SER	2.4
2	U	51	ILE	2.4
2	J	153	GLY	2.4
2	F	109	PHE	2.4
3	g	112	PRO	2.4
3	g	184	THR	2.4
1	B	160	TYR	2.4
1	Q	64	LEU	2.4
3	g	181	LEU	2.4
1	B	1	SER	2.4
3	N	126	GLU	2.4
2	Y	112	TRP	2.4
1	B	245	ARG	2.4
3	h	198	VAL	2.4
3	g	180	TYR	2.4
1	B	243	PRO	2.3
1	E	230	VAL	2.3
3	h	194	TYR	2.3
2	F	152	LYS	2.3
1	Q	112	ILE	2.3
3	f	134	THR	2.3
3	O	50	ILE	2.3
1	P	39	ILE	2.3
2	Y	192	VAL	2.3
1	E	243	PRO	2.3
2	Y	176	PRO	2.3
3	g	121	PHE	2.3
2	Y	45	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	Y	46	GLU	2.3
3	M	176	MET	2.3
3	h	196	CYS	2.3
3	Z	77	ILE	2.3
1	E	254	LEU	2.2
1	T	219	GLN	2.2
1	D	230	VAL	2.2
1	E	233	VAL	2.2
1	Q	277	ASP	2.2
1	T	220	LEU	2.2
1	S	264	ASN	2.2
1	E	250	VAL	2.2
2	V	132	PRO	2.2
2	J	220	VAL	2.2
3	f	135	LEU	2.2
3	M	137	CYS	2.2
2	F	202	VAL	2.2
2	Y	105	TYR	2.2
2	J	218	LYS	2.2
1	D	1	SER	2.2
1	P	227	LEU	2.2
3	h	180	TYR	2.2
3	h	137	CYS	2.2
1	E	304	GLY	2.2
2	G	152	LYS	2.2
2	V	187	SER	2.2
2	V	186	LEU	2.1
3	g	49	LEU	2.1
1	E	240	THR	2.1
3	K	129	GLU	2.1
1	E	44	VAL	2.1
3	g	10	LEU	2.1
1	E	277	ASP	2.1
2	U	70	LEU	2.1
3	N	181	LEU	2.1
3	g	105	LYS	2.1
2	V	206	VAL	2.1
2	I	149	CYS	2.1
1	R	244	ALA	2.1
2	I	147	LEU	2.1
2	G	135	PRO	2.1
1	P	1	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	N	38	VAL	2.1
2	X	147	LEU	2.1
2	Y	20	ILE	2.1
3	Z	84	ASP	2.1
3	K	121	PHE	2.1
3	M	119	THR	2.1
3	M	120	LEU	2.1
2	W	132	PRO	2.1
2	U	207	ALA	2.1
2	G	149	CYS	2.1
2	U	29	PHE	2.0
1	P	112	ILE	2.0
2	V	219	ILE	2.0
1	B	152	ALA	2.0
1	E	284	MET	2.0
3	M	183	LEU	2.0
2	J	173	HIS	2.0
3	L	132	LYS	2.0
2	X	145	VAL	2.0
1	B	139	MET	2.0
1	R	291	LEU	2.0
2	G	185	THR	2.0
1	B	153	TYR	2.0
2	F	59	SER	2.0
1	S	248	LEU	2.0
2	W	133	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	LMT	R	402	23/35	0.68	0.37	0.50	149,149,149,149	0
5	LMT	T	402	25/35	0.80	0.34	0.17	145,145,145,145	0
5	LMT	B	402	23/35	0.70	0.36	0.17	181,181,181,181	0
5	LMT	C	402	23/35	0.67	0.33	0.15	173,173,173,173	0
5	LMT	A	402	23/35	0.65	0.24	-0.00	211,211,211,211	0
5	LMT	D	402	23/35	0.77	0.32	-0.04	189,189,189,189	0
5	LMT	P	402	23/35	0.79	0.28	-0.37	149,149,149,149	0
5	LMT	E	402	23/35	0.75	0.25	-0.77	177,177,177,177	0
5	LMT	S	402	23/35	0.83	0.23	-1.55	130,130,130,130	0
5	LMT	Q	402	23/35	0.76	0.18	-1.93	143,143,143,143	0
6	FLC	A	403	13/13	0.88	0.35	-	168,168,168,168	0
4	NAG	C	401	14/15	0.84	0.20	-	158,158,158,158	0
4	NAG	S	401	14/15	0.85	0.38	-	218,218,218,218	0
4	NAG	T	401	14/15	0.84	0.19	-	182,182,182,182	0
4	NAG	R	401	14/15	0.91	0.16	-	191,191,191,191	0
7	CL	P	404	1/1	0.91	2.54	-	115,115,115,115	0
4	NAG	P	401	14/15	0.81	0.53	-	232,232,232,232	0
6	FLC	T	403	13/13	0.81	0.38	-	187,187,187,187	0
4	NAG	D	401	14/15	0.84	0.20	-	204,204,204,204	0
4	NAG	B	401	14/15	0.90	0.15	-	172,172,172,172	0
4	NAG	E	401	14/15	0.90	0.14	-	170,170,170,170	0
7	CL	P	403	1/1	0.77	1.88	-	115,115,115,115	0
4	NAG	Q	401	14/15	0.79	0.27	-	176,176,176,176	0
4	NAG	A	401	14/15	0.91	0.16	-	165,165,165,165	0

6.5 Other polymers (i)

There are no such residues in this entry.