Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2014 – 09:00 PM EDT

PDB ID	:	4TNW
Title	:	C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab and POPC in a lipid-modulated conformation
Authors	:	Althoff, T.; Hibbs, R.E.; Banerjee, S.; Gouaux, E.
Deposited on	:	2014-06-05
Resolution	:	3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html

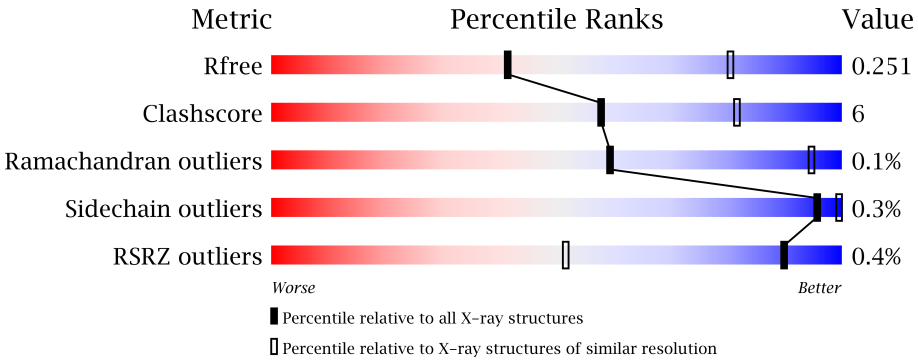
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23489
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	
1	E	347	
1	P	347	
1	Q	347	
1	R	347	
1	S	347	
1	T	347	
2	F	224	
2	G	224	
2	H	224	
2	I	224	

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Mol	Chain	Length	Quality of chain
2	J	224	
2	U	224	
2	V	224	
2	W	224	
2	X	224	
2	Y	224	
3	K	215	
3	L	215	
3	M	215	
3	N	215	
3	O	215	
3	Z	215	
3	f	215	
3	g	215	
3	h	215	
3	i	215	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	E	401	-	X
4	NAG	S	401	-	X
4	NAG	T	402	-	X
5	POV	A	402	-	X
5	POV	D	401	-	X
5	POV	P	403	-	X
5	POV	Q	401	-	X
5	POV	R	401	-	X
5	POV	R	402	-	X
5	POV	T	401	-	X
8	LMT	D	403	-	X
8	LMT	E	402	-	X
8	LMT	S	402	-	X
8	LMT	T	403	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 60818 atoms, of which 0 are hydrogen and 0 are deuterium.

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	342	Total	C	N	O	S	0	0	0
			2744	1786	449	494	15			
1	B	341	Total	C	N	O	S	0	0	0
			2734	1780	446	493	15			
1	C	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	D	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	E	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	P	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	Q	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	R	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	S	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	T	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	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

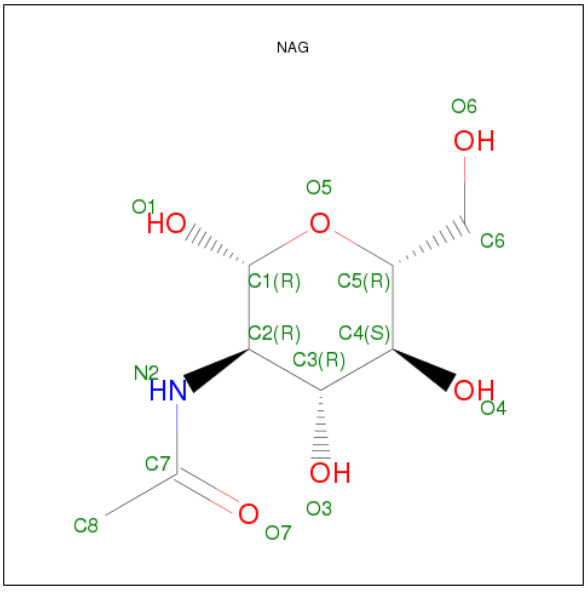
- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	221	Total	C	N	O	S	0	0	0
			1682	1067	273	334	8			
2	G	222	Total	C	N	O	S	0	0	0
			1693	1073	277	335	8			
2	H	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			
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	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.

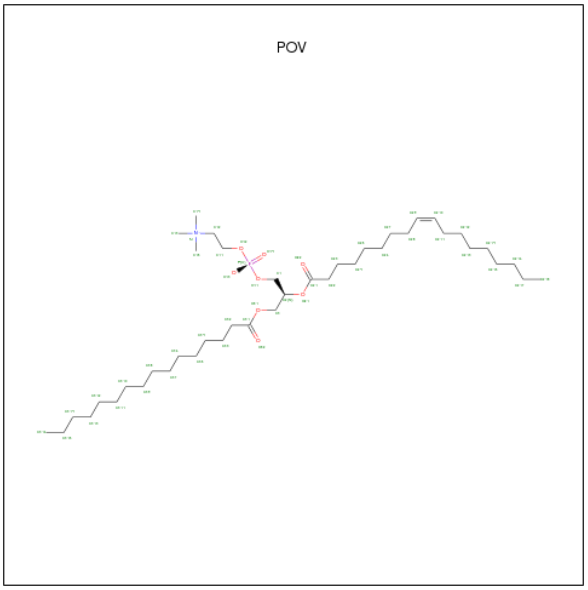
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	210	Total	C	N	O	S	0	0	0
			1590	999	266	319	6			
3	L	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	N	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	O	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	Z	215	Total	C	N	O	S	0	0	0
			1626	1018	274	327	7			
3	f	215	Total	C	N	O	S	0	0	0
			1626	1018	274	327	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	210	Total	C	N	O	S	0	0	0
			1590	999	266	319	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	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 (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl2-(trimethylammonio)ethylphosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			23	14	1	7	1		
5	D	1	Total	C	N	O	P	0	0
			26	16	1	8	1		

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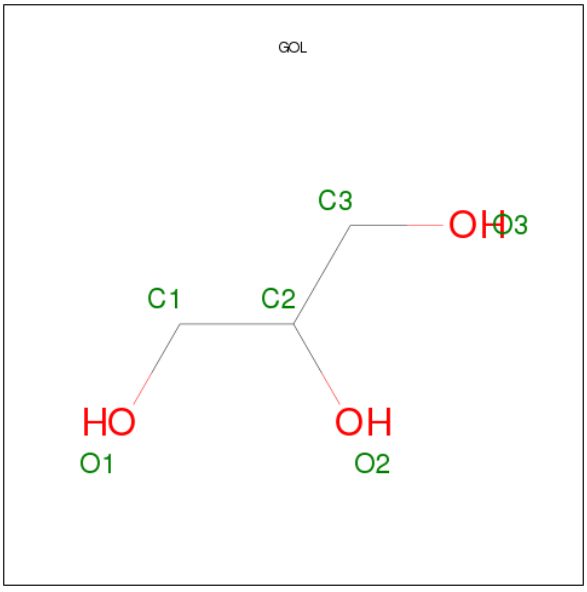
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total C N O P 42 32 1 8 1	0	0
5	Q	1	Total C N O P 46 36 1 8 1	0	0
5	R	1	Total C N O P 34 24 1 8 1	0	0
5	R	1	Total C O P 35 26 8 1	0	0
5	T	1	Total C N O P 43 33 1 8 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0

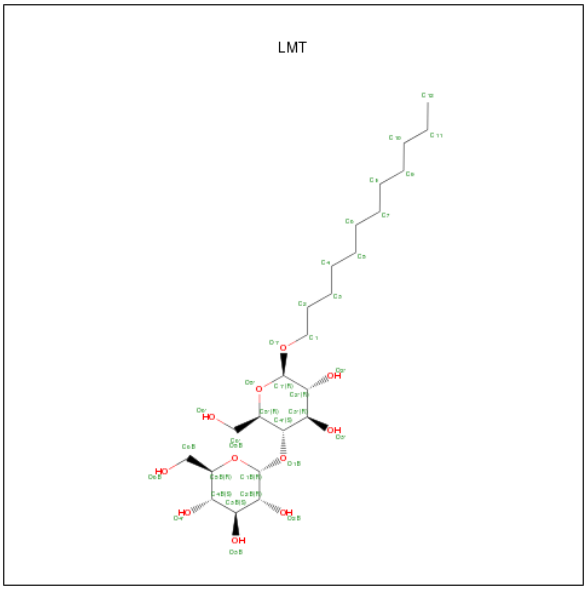
- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 6 3 3	0	0

- Molecule 8 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:

$C_{24}H_{46}O_{11}$).



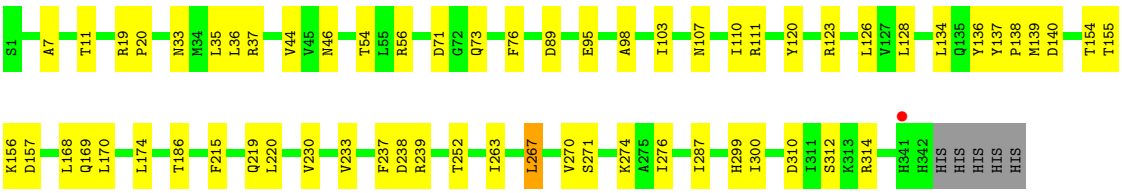
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			23	12	11		
8	C	1	Total	C	O	0	0
			23	12	11		
8	D	1	Total	C	O	0	0
			23	12	11		
8	E	1	Total	C	O	0	0
			23	12	11		
8	P	1	Total	C	O	0	0
			23	12	11		
8	S	1	Total	C	O	0	0
			23	12	11		
8	T	1	Total	C	O	0	0
			23	12	11		

3 Residue-property plots

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.

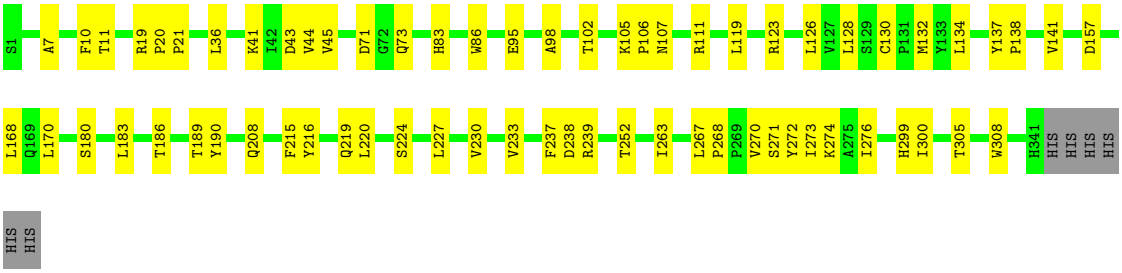
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain A:



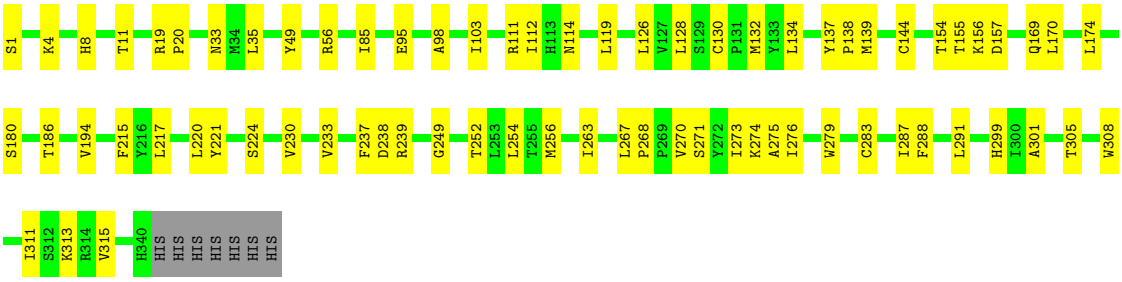
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain B:



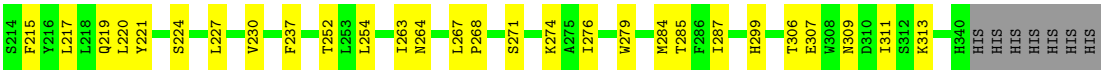
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain C:



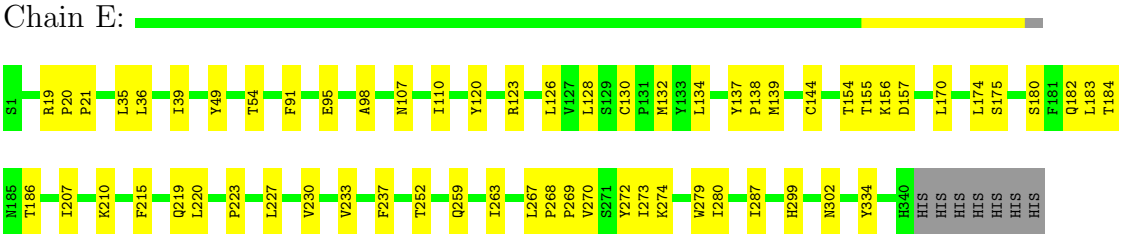
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain D:



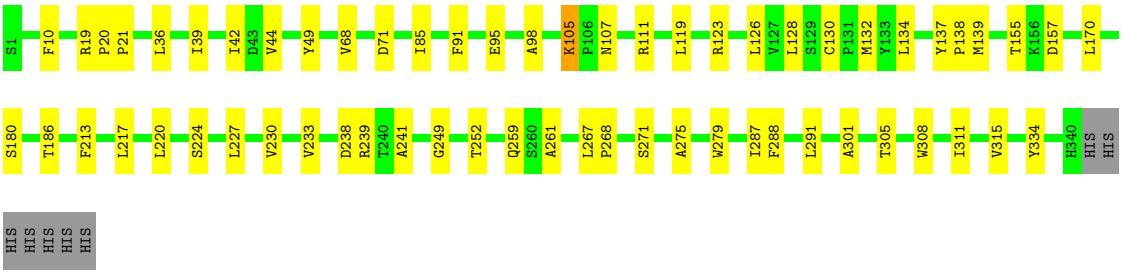
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain E:



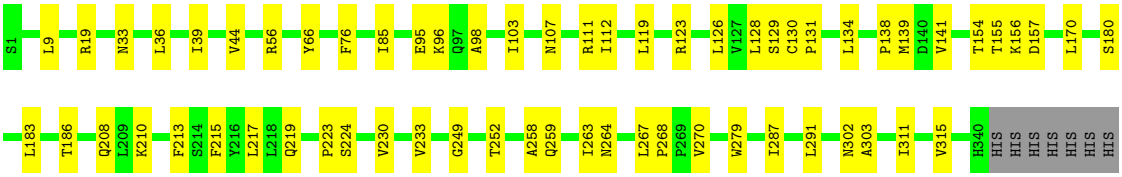
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain P:



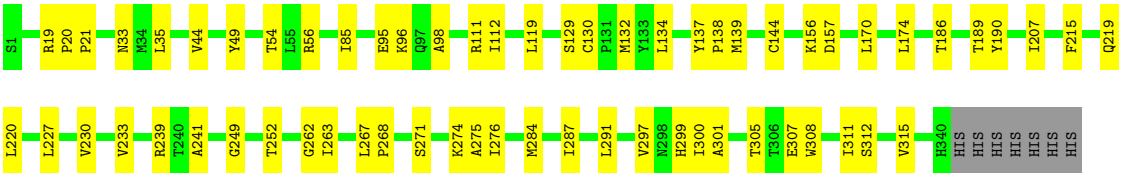
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain Q:



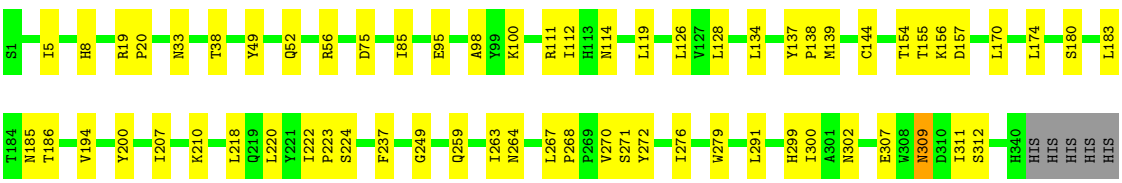
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain R:



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

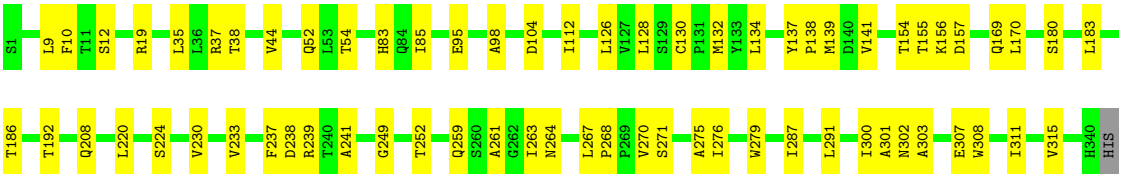
Chain S:



HIS
HIS

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

Chain T:



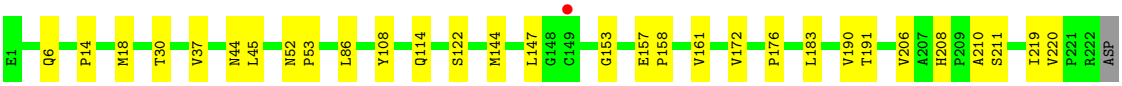
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain F:

• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

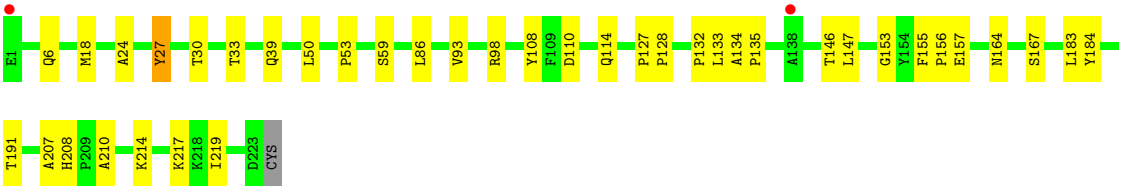
Chain G:



CYS

• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain H:

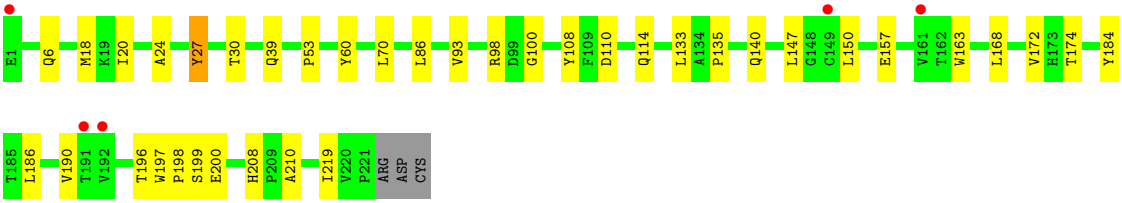


• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain I:

• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain U:

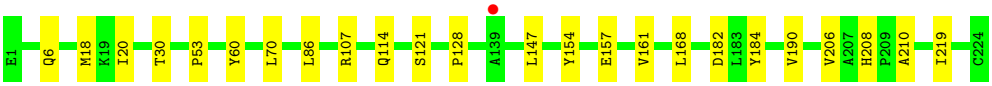


• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain V:

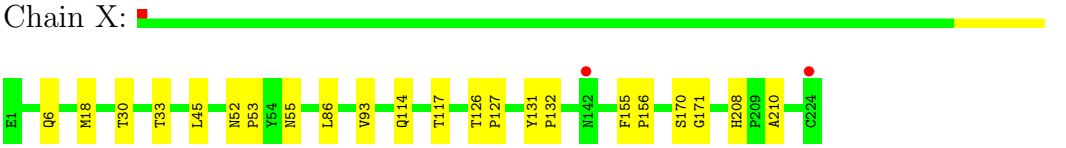
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain W:



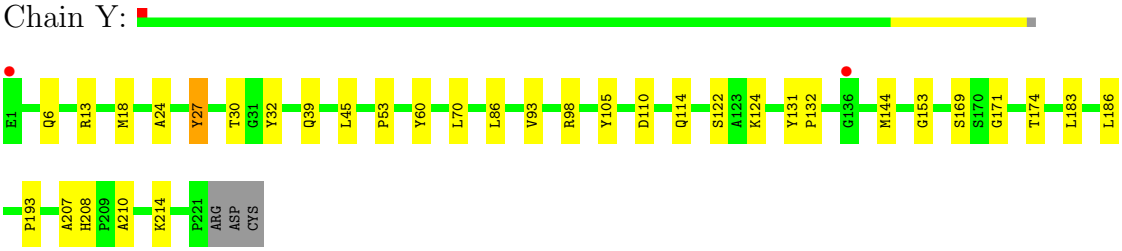
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain X:



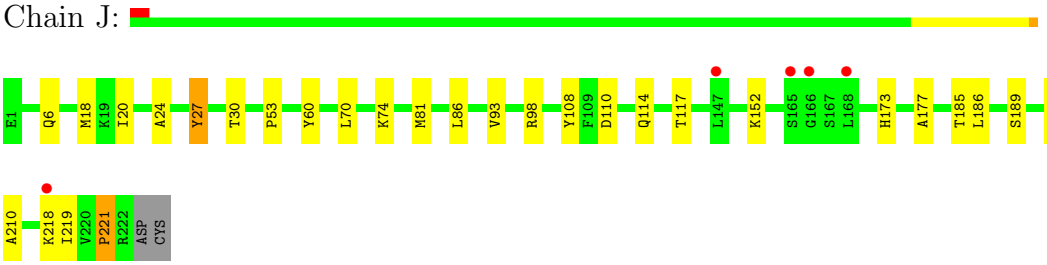
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain Y:



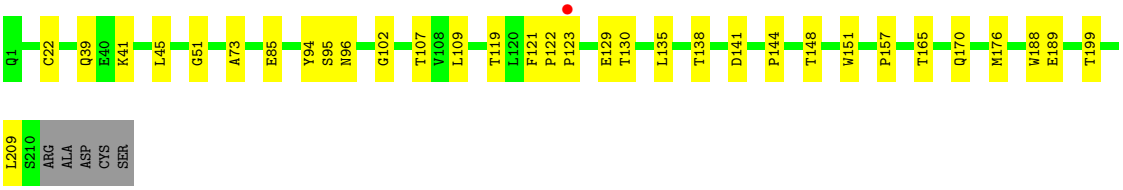
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain J:



• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain K:

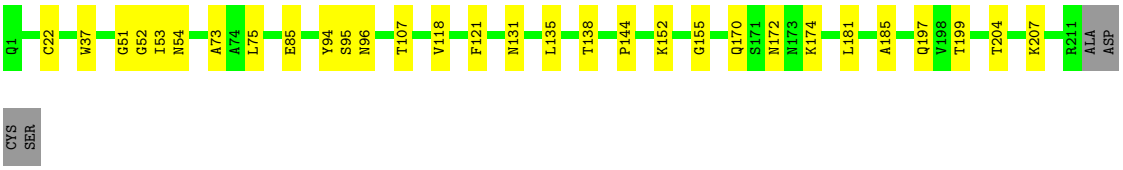


• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain L:

• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain N:

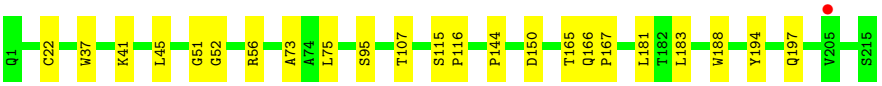


• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain O:

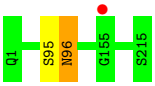
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain Z:



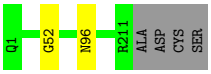
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain f:



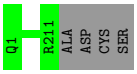
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain g:



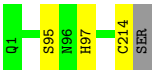
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain h:



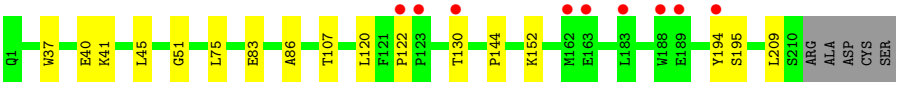
• Molecule 3: Mouse monoclonal Fab fragment, light chain

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	453.75Å 192.87Å 196.14Å 90.00° 92.27° 90.00°	Depositor
Resolution (Å)	58.70 – 3.20 59.51 – 3.00	Depositor EDS
% Data completeness (in resolution range)	77.6 (58.70-3.20) 88.8 (59.51-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.227 , 0.251 0.230 , 0.251	Depositor DCC
R_{free} test set	12804 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	84.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 48.2	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 297382 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	60818	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, GOL, 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	0.24	0/2819	0.44	0/3847
1	B	0.23	0/2808	0.43	0/3832
1	C	0.23	0/2797	0.43	0/3817
1	D	0.25	0/2797	0.48	0/3817
1	E	0.24	0/2797	0.44	0/3817
1	P	0.24	0/2797	0.45	0/3817
1	Q	0.24	0/2797	0.45	0/3817
1	R	0.24	0/2797	0.43	0/3817
1	S	0.23	0/2797	0.43	0/3817
1	T	0.24	0/2797	0.45	0/3817
2	F	0.21	0/1728	0.40	0/2360
2	G	0.22	0/1739	0.41	0/2374
2	H	0.22	0/1747	0.41	0/2385
2	I	0.21	0/1739	0.40	0/2374
2	J	0.23	0/1739	0.42	0/2374
2	U	0.21	0/1728	0.40	0/2360
2	V	0.21	0/1753	0.40	0/2393
2	W	0.21	0/1753	0.40	0/2393
2	X	0.22	0/1753	0.42	0/2393
2	Y	0.21	0/1728	0.41	0/2360
3	K	0.22	0/1628	0.42	0/2226
3	L	0.22	0/1639	0.43	0/2240
3	M	0.22	0/1628	0.43	0/2226
3	N	0.23	0/1639	0.43	0/2240
3	O	0.22	0/1639	0.42	0/2240
3	Z	0.23	0/1664	0.43	0/2274
3	f	0.22	0/1664	0.42	0/2274
3	g	0.22	0/1639	0.42	0/2240
3	h	0.22	0/1639	0.41	0/2240
3	i	0.22	0/1658	0.43	0/2266
All	All	0.23	0/61847	0.43	0/84447

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2744	0	2744	45	0
1	B	2734	0	2737	48	0
1	C	2724	0	2729	51	0
1	D	2724	0	2729	45	0
1	E	2724	0	2730	46	0
1	P	2724	0	2730	41	0
1	Q	2724	0	2730	41	0
1	R	2724	0	2731	43	0
1	S	2724	0	2730	50	0
1	T	2724	0	2730	49	0
2	F	1682	0	1632	24	0
2	G	1693	0	1645	20	0
2	H	1701	0	1649	26	0
2	I	1693	0	1645	23	0
2	J	1693	0	1645	23	0
2	U	1682	0	1632	22	0
2	V	1707	0	1653	20	0
2	W	1707	0	1653	14	0
2	X	1707	0	1653	13	0
2	Y	1682	0	1632	21	0
3	K	1590	0	1542	23	0
3	L	1601	0	1555	19	0
3	M	1590	0	1542	11	0
3	N	1601	0	1555	21	0
3	O	1601	0	1555	16	0
3	Z	1626	0	1573	13	0
3	f	1626	0	1573	0	0
3	g	1601	0	1555	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	h	1601	0	1555	0	0
3	i	1620	0	1568	0	0
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	S	14	0	13	1	0
4	T	14	0	13	0	0
5	A	23	0	26	1	0
5	D	26	0	26	5	0
5	P	42	0	61	3	0
5	Q	46	0	67	5	0
5	R	69	0	83	5	0
5	T	43	0	63	3	0
6	A	1	0	0	0	0
6	P	1	0	0	0	0
7	B	6	0	8	0	0
8	B	23	0	21	0	0
8	C	23	0	21	0	0
8	D	23	0	21	1	0
8	E	23	0	21	0	0
8	P	23	0	21	0	0
8	S	23	0	21	1	0
8	T	23	0	21	1	0
All	All	60818	0	59930	703	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (703) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:306:THR:HA	1:D:309:ASN:HB2	1.53	0.90
1:Q:302:ASN:HD22	1:R:241:ALA:HB2	1.36	0.89
1:T:37:ARG:NH2	1:T:54:THR:OG1	2.10	0.84
1:C:305:THR:HG22	1:C:308:TRP:HD1	1.43	0.83
1:R:156:LYS:HA	3:Z:95:SER:HB2	1.61	0.83
1:D:156:LYS:HA	3:O:95:SER:HB2	1.61	0.81
2:Y:13:ARG:HH22	2:Y:124:LYS:HD2	1.46	0.81
1:Q:302:ASN:ND2	1:R:241:ALA:HB2	1.96	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:37:ARG:NH1	1:D:54:THR:OG1	2.17	0.78
1:Q:141:VAL:HG22	1:Q:210:LYS:HG2	1.67	0.76
1:P:241:ALA:HB2	1:T:302:ASN:HD22	1.52	0.75
1:P:91:PHE:HA	1:Q:103:ILE:HD11	1.69	0.75
1:B:220:LEU:HD22	1:B:263:ILE:HG13	1.68	0.74
3:M:194:TYR:HB2	3:M:209:LEU:HB3	1.69	0.74
1:B:44:VAL:HG11	1:B:134:LEU:HD11	1.69	0.74
1:T:10:PHE:HE2	1:T:83:HIS:HB3	1.52	0.74
1:Q:44:VAL:HG11	1:Q:134:LEU:HD11	1.69	0.73
3:M:107:THR:HG21	3:M:144:PRO:HB3	1.73	0.71
1:Q:267:LEU:HD12	1:Q:268:PRO:HD2	1.72	0.70
1:B:71:ASP:OD2	1:B:73:GLN:NE2	2.23	0.70
1:C:305:THR:HG22	1:C:308:TRP:CD1	2.25	0.70
1:P:267:LEU:HD12	1:P:268:PRO:HD2	1.73	0.69
2:F:152:LYS:HB2	2:F:195:SER:HB2	30.38	0.69
2:V:153:GLY:HA2	2:V:183:LEU:HB3	1.73	0.69
2:I:6:GLN:H	2:I:114:GLN:HE22	1.41	0.69
2:V:6:GLN:H	2:V:114:GLN:HE22	1.40	0.69
1:T:267:LEU:HD12	1:T:268:PRO:HD2	1.74	0.68
1:R:267:LEU:HD12	1:R:268:PRO:HD2	1.74	0.68
1:S:111:ARG:HD2	1:S:119:LEU:HD23	1.76	0.68
2:I:108:TYR:HB2	3:O:51:GLY:HA3	1.74	0.68
2:V:108:TYR:HB2	3:Z:51:GLY:HA3	1.76	0.68
1:A:238:ASP:OD1	1:A:239:ARG:N	2.27	0.68
1:T:10:PHE:CE2	1:T:83:HIS:HB3	2.28	0.68
2:J:219:ILE:HG22	2:J:221:PRO:HD3	1.76	0.67
2:W:6:GLN:H	2:W:114:GLN:HE22	1.42	0.67
1:S:210:LYS:NZ	8:S:402:LMT:O4'	2.27	0.67
2:G:108:TYR:HB2	3:K:51:GLY:HA3	1.77	0.67
2:J:108:TYR:HB2	3:M:51:GLY:HA3	1.76	0.67
3:K:107:THR:HG21	3:K:144:PRO:HB3	1.76	0.67
1:C:267:LEU:HD21	1:C:274:LYS:HE3	1.77	0.67
2:H:108:TYR:HB2	3:L:51:GLY:HA3	1.78	0.66
1:E:186:THR:HG22	1:E:207:ILE:HG22	1.78	0.66
1:D:267:LEU:HD11	1:D:274:LYS:HE3	1.78	0.66
5:D:401:POV:O13	1:E:259:GLN:NE2	2.28	0.66
1:A:37:ARG:NH1	1:A:54:THR:OG1	2.29	0.66
1:Q:249:GLY:HA3	1:Q:291:LEU:HD13	1.78	0.66
2:U:6:GLN:H	2:U:114:GLN:HE22	1.43	0.66
1:A:103:ILE:HG21	1:E:98:ALA:HB3	1.78	0.66
1:E:134:LEU:HD12	1:E:270:VAL:HG21	1.78	0.66
3:O:135:LEU:HD12	3:O:181:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:238:ASP:OD1	1:T:239:ARG:N	2.28	0.65
2:J:173:HIS:HB2	2:J:189:SER:HB2	1.78	0.65
3:N:107:THR:HG21	3:N:144:PRO:HB3	1.78	0.65
2:V:134:ALA:HB3	2:V:222:ARG:HG3	1.78	0.65
2:W:30:THR:HA	2:W:53:PRO:HB2	1.78	0.65
1:B:267:LEU:HD21	1:B:274:LYS:HE3	1.78	0.65
3:K:41:LYS:HB2	3:K:45:LEU:HB3	1.77	0.65
1:Q:36:LEU:HD21	1:Q:39:ILE:HD11	1.78	0.65
1:R:44:VAL:HG11	1:R:134:LEU:HD11	1.78	0.65
1:D:307:GLU:O	1:D:311:ILE:HG13	1.96	0.64
1:C:220:LEU:HD22	1:C:263:ILE:HG13	1.78	0.64
1:T:249:GLY:HA3	1:T:291:LEU:HD13	1.79	0.64
1:A:238:ASP:OD2	1:E:302:ASN:ND2	2.31	0.64
2:G:6:GLN:H	2:G:114:GLN:HE22	1.44	0.64
1:T:300:ILE:HG23	1:T:308:TRP:HE3	1.62	0.64
2:J:6:GLN:H	2:J:114:GLN:HE22	1.45	0.64
2:H:6:GLN:H	2:H:114:GLN:HE22	1.46	0.64
2:Y:6:GLN:H	2:Y:114:GLN:HE22	1.44	0.63
1:P:238:ASP:OD1	1:P:239:ARG:N	2.31	0.63
1:B:10:PHE:CE2	1:B:83:HIS:HB3	2.33	0.63
1:P:44:VAL:HG11	1:P:134:LEU:HD11	1.80	0.63
5:D:401:POV:H3A	1:E:223:PRO:HB3	1.79	0.62
1:B:238:ASP:OD1	1:B:239:ARG:N	2.32	0.62
2:F:144:MET:HB2	2:F:191:THR:HG22	1.81	0.62
2:I:222:ARG:NH2	3:O:123:PRO:O	2.32	0.62
3:O:96:ASN:O	3:O:96:ASN:ND2	2.28	0.62
2:F:6:GLN:H	2:F:114:GLN:HE22	1.45	0.62
3:L:107:THR:HG21	3:L:144:PRO:HB3	1.82	0.61
1:T:19:ARG:HH11	1:T:157:ASP:HA	1.65	0.61
2:I:30:THR:HA	2:I:53:PRO:HB2	1.82	0.61
1:Q:141:VAL:HG11	1:Q:208:GLN:HE21	1.66	0.61
1:P:180:SER:HA	1:T:271:SER:HB2	1.81	0.61
1:A:36:LEU:HD13	1:A:168:LEU:HD11	1.82	0.61
1:S:154:THR:OG1	1:S:155:THR:N	2.34	0.61
1:S:267:LEU:HD12	1:S:268:PRO:HD2	1.83	0.61
3:K:22:CYS:HB3	3:K:73:ALA:HB3	1.82	0.61
2:Y:24:ALA:HB1	2:Y:27:TYR:HE1	1.66	0.61
1:D:44:VAL:HG21	1:D:268:PRO:HG3	1.82	0.61
1:C:170:LEU:HD23	1:C:174:LEU:HD23	1.82	0.60
2:V:30:THR:HA	2:V:53:PRO:HB2	1.83	0.60
2:H:33:THR:HG21	2:H:50:LEU:HD12	1.84	0.60
2:I:98:ARG:NH2	2:I:110:ASP:OD2	2.27	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:VAL:HG11	1:A:134:LEU:HD11	1.83	0.60
1:D:213:PHE:CE2	1:D:217:LEU:HD12	2.37	0.60
1:D:220:LEU:HD22	1:D:263:ILE:HG13	1.83	0.60
2:F:98:ARG:NH2	2:F:110:ASP:OD2	2.29	0.60
1:E:267:LEU:HD21	1:E:274:LYS:HE3	1.84	0.59
1:A:134:LEU:HD12	1:A:270:VAL:HG21	1.83	0.59
1:T:35:LEU:HB3	1:T:54:THR:HB	1.84	0.59
2:Y:24:ALA:HB1	2:Y:27:TYR:CE1	2.38	0.59
2:I:24:ALA:HB1	2:I:27:TYR:HE1	1.67	0.59
1:R:170:LEU:HD23	1:R:174:LEU:HD23	1.85	0.58
1:S:218:LEU:HD23	1:S:222:ILE:HG13	1.83	0.58
1:P:155:THR:OG1	2:W:107:ARG:NH2	2.37	0.58
3:N:94:TYR:O	3:N:96:ASN:N	2.36	0.58
2:H:147:LEU:HD13	2:H:219:ILE:HG13	1.84	0.58
2:Y:30:THR:HA	2:Y:53:PRO:HB2	1.86	0.58
1:P:249:GLY:HA3	1:P:291:LEU:HD13	1.85	0.58
1:S:134:LEU:HD12	1:S:270:VAL:HG21	1.86	0.58
1:D:7:ALA:O	1:D:11:THR:HG23	2.04	0.58
1:C:98:ALA:HB3	1:D:103:ILE:HG13	1.85	0.57
2:H:98:ARG:NH2	2:H:110:ASP:OD2	2.33	0.57
1:T:9:LEU:O	1:T:12:SER:OG	2.21	0.57
3:K:39:GLN:NE2	3:K:41:LYS:HE3	2.18	0.57
1:R:239:ARG:NH1	1:R:301:ALA:HB1	2.19	0.57
1:D:19:ARG:HH11	1:D:157:ASP:HA	1.69	0.57
3:L:135:LEU:HB2	3:L:181:LEU:HB3	1.86	0.57
1:A:7:ALA:O	1:A:11:THR:HG23	2.03	0.57
1:B:36:LEU:HD13	1:B:168:LEU:HD11	1.85	0.57
1:C:238:ASP:OD1	1:C:239:ARG:N	2.37	0.57
2:G:30:THR:HA	2:G:53:PRO:HB2	1.85	0.57
1:P:107:ASN:OD1	1:P:123:ARG:NH1	2.38	0.57
1:P:227:LEU:HD13	5:P:403:POV:H22A	1.87	0.57
3:Z:41:LYS:HB2	3:Z:45:LEU:HB2	1.86	0.57
2:X:93:VAL:HG22	2:X:117:THR:HG22	1.86	0.57
3:N:135:LEU:HB2	3:N:181:LEU:HB3	1.87	0.57
2:W:128:PRO:HB3	2:W:154:TYR:HB3	1.86	0.56
2:X:30:THR:HA	2:X:53:PRO:HB2	1.86	0.56
2:F:27:TYR:CE2	2:F:98:ARG:HD2	2.41	0.56
2:H:24:ALA:HB1	2:H:27:TYR:HE1	1.68	0.56
3:M:41:LYS:HB2	3:M:45:LEU:HB2	1.87	0.56
1:C:154:THR:OG1	1:C:155:THR:N	2.38	0.56
3:N:152:LYS:HE3	3:N:155:GLY:HA2	1.86	0.56
1:Q:9:LEU:HD11	1:Q:66:TYR:HB3	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:ARG:HD3	1:A:312:SER:HB3	1.87	0.56
1:B:98:ALA:HB3	1:C:103:ILE:HG13	1.88	0.56
1:T:154:THR:OG1	1:T:155:THR:N	2.38	0.56
1:A:156:LYS:HA	3:L:95:SER:HB2	1.87	0.56
2:V:13:ARG:NH2	2:V:123:ALA:O	2.39	0.56
1:Q:258:ALA:HB1	5:Q:401:POV:H13B	1.87	0.56
1:Q:154:THR:OG1	1:Q:155:THR:N	2.38	0.55
1:T:220:LEU:HD22	1:T:263:ILE:HG13	1.87	0.55
2:U:30:THR:HA	2:U:53:PRO:HB2	1.89	0.55
2:F:24:ALA:HB1	2:F:27:TYR:HE1	1.69	0.55
2:J:93:VAL:HG22	2:J:117:THR:HG22	1.87	0.55
1:P:36:LEU:HD21	1:P:39:ILE:HD11	1.87	0.55
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.42	0.55
1:B:271:SER:HB2	1:C:180:SER:HA	1.89	0.55
1:T:302:ASN:OD1	1:T:303:ALA:N	2.40	0.55
2:X:6:GLN:H	2:X:114:GLN:HE22	1.53	0.55
1:A:126:LEU:HD13	1:A:128:LEU:HD21	1.87	0.55
1:A:219:GLN:NE2	5:A:402:POV:H12	2.21	0.55
2:J:98:ARG:NH2	2:J:110:ASP:OD2	2.32	0.55
2:U:60:TYR:HE1	2:U:70:LEU:HG	1.72	0.55
2:I:24:ALA:HB1	2:I:27:TYR:CE1	2.41	0.55
1:P:42:ILE:HG12	1:P:49:TYR:HB2	1.87	0.55
1:T:44:VAL:HG11	1:T:134:LEU:HD11	1.88	0.55
2:U:172:VAL:HA	2:U:190:VAL:HG12	1.87	0.55
1:Q:111:ARG:HD2	1:Q:119:LEU:HD23	1.89	0.55
1:R:137:TYR:HB3	1:R:274:LYS:HB3	1.88	0.55
1:B:107:ASN:OD1	1:B:123:ARG:NH1	2.39	0.55
1:E:184:THR:HG21	1:E:210:LYS:HD2	1.88	0.55
3:O:94:TYR:HB2	3:O:97:HIS:HB3	1.89	0.54
1:R:111:ARG:HD2	1:R:119:LEU:HD23	1.89	0.54
2:Y:39:GLN:HB3	2:Y:93:VAL:HG13	1.89	0.54
1:B:141:VAL:HG11	1:B:208:GLN:HE21	1.73	0.54
1:E:154:THR:OG1	1:E:155:THR:N	2.40	0.54
1:P:95:GLU:HG3	1:P:98:ALA:HB2	1.88	0.54
2:V:108:TYR:CB	3:Z:51:GLY:HA3	2.37	0.54
1:D:220:LEU:HD23	1:D:276:ILE:HD11	1.90	0.54
1:E:126:LEU:HD13	1:E:128:LEU:HD21	1.89	0.54
1:P:261:ALA:HA	5:Q:401:POV:H14B	1.90	0.54
2:G:172:VAL:HA	2:G:190:VAL:HG12	1.90	0.54
1:P:19:ARG:HH11	1:P:157:ASP:HA	1.73	0.54
1:C:252:THR:HG22	1:C:287:ILE:HD13	1.88	0.54
1:E:252:THR:HG22	1:E:287:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:284:MET:HG2	5:D:401:POV:H1	1.88	0.54
1:A:103:ILE:HD11	1:E:91:PHE:HA	1.90	0.54
1:E:95:GLU:HG3	1:E:98:ALA:HB2	1.89	0.54
1:D:139:MET:HG2	8:D:403:LMT:H6D	1.90	0.53
1:S:249:GLY:HA3	1:S:291:LEU:HD13	1.90	0.53
1:D:95:GLU:HG3	1:D:98:ALA:HB2	1.89	0.53
3:K:170:GLN:HE21	3:K:176:MET:HB3	1.73	0.53
1:Q:302:ASN:OD1	1:Q:303:ALA:N	2.42	0.53
1:T:85:ILE:HD11	1:T:112:ILE:HD11	1.90	0.53
1:D:167:PRO:HB2	1:D:188:THR:HG21	1.90	0.53
3:L:152:LYS:HB2	3:L:195:SER:HB3	1.90	0.53
2:U:24:ALA:HB1	2:U:27:TYR:HE1	1.73	0.53
1:C:85:ILE:HD11	1:C:112:ILE:HD11	1.90	0.53
2:G:108:TYR:CB	3:K:51:GLY:HA3	2.38	0.53
3:O:135:LEU:HB2	3:O:181:LEU:HB3	1.90	0.53
1:A:95:GLU:HG3	1:A:98:ALA:HB2	1.90	0.53
1:E:107:ASN:OD1	1:E:123:ARG:NH1	2.41	0.53
3:K:119:THR:OG1	3:K:138:THR:OG1	2.26	0.53
1:C:126:LEU:HD13	1:C:128:LEU:HD21	1.91	0.53
3:K:123:PRO:HD3	3:K:135:LEU:HG	1.91	0.53
2:Y:98:ARG:NH2	2:Y:110:ASP:OD2	2.40	0.53
1:D:267:LEU:HD12	1:D:268:PRO:HD2	1.90	0.53
1:B:134:LEU:HD12	1:B:270:VAL:HG21	1.91	0.53
5:D:401:POV:P	1:E:259:GLN:HE22	2.32	0.53
1:A:154:THR:OG1	1:A:155:THR:N	2.38	0.52
3:O:85:GLU:HG3	3:O:107:THR:HA	1.89	0.52
1:B:126:LEU:HD13	1:B:128:LEU:HD21	1.90	0.52
1:A:71:ASP:OD2	1:A:73:GLN:NE2	2.29	0.52
2:J:108:TYR:CB	3:M:51:GLY:HA3	2.39	0.52
2:F:108:TYR:HB2	3:N:51:GLY:HA2	1.91	0.52
2:V:132:PRO:HG3	2:V:217:LYS:HB3	1.92	0.52
1:A:46:ASN:ND2	1:B:41:LYS:HE2	2.25	0.52
2:H:30:THR:HA	2:H:53:PRO:HB2	1.91	0.52
1:S:126:LEU:HD13	1:S:128:LEU:HD21	1.92	0.52
3:N:131:ASN:HA	3:N:185:ALA:HB2	1.92	0.52
1:T:134:LEU:HD12	1:T:270:VAL:HG21	1.92	0.52
1:A:220:LEU:HD22	1:A:263:ILE:HG13	1.92	0.51
1:A:267:LEU:HD11	1:A:274:LYS:HE3	1.91	0.51
2:H:207:ALA:HB2	2:H:214:LYS:HD3	1.92	0.51
2:H:39:GLN:HB3	2:H:93:VAL:HG13	1.92	0.51
1:Q:252:THR:HG22	1:Q:287:ILE:HD13	1.92	0.51
3:Z:37:TRP:CE2	3:Z:75:LEU:HB2	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:V:176:PRO:HG2	3:Z:165:THR:HB	1.92	0.51
1:C:249:GLY:HA3	1:C:291:LEU:HD13	1.92	0.51
1:E:138:PRO:HD2	1:E:139:MET:SD	2.50	0.51
2:G:147:LEU:HD13	2:G:219:ILE:HD13	1.93	0.51
2:I:6:GLN:N	2:I:114:GLN:HE22	2.08	0.51
1:R:239:ARG:HH11	1:R:301:ALA:HB1	1.76	0.51
1:S:220:LEU:HD22	1:S:263:ILE:HG13	1.92	0.51
1:T:263:ILE:HG21	1:T:276:ILE:HG12	1.93	0.51
2:U:39:GLN:HB3	2:U:93:VAL:HG13	1.92	0.51
2:F:24:ALA:HB1	2:F:27:TYR:CE1	2.45	0.51
1:P:213:PHE:CE2	1:P:217:LEU:HD12	2.45	0.51
1:Q:213:PHE:CE2	1:Q:217:LEU:HD12	2.45	0.51
2:J:30:THR:HA	2:J:53:PRO:HB2	1.93	0.51
3:L:37:TRP:CE2	3:L:75:LEU:HB2	2.45	0.51
1:P:105:LYS:N	1:P:105:LYS:HD2	2.26	0.51
1:Q:170:LEU:HD11	1:Q:186:THR:HG21	1.93	0.51
1:T:252:THR:HG22	1:T:287:ILE:HD13	1.93	0.51
1:A:89:ASP:HB2	1:B:105:LYS:HD3	1.93	0.51
1:C:95:GLU:HG3	1:C:98:ALA:HB2	1.92	0.51
3:L:22:CYS:HB3	3:L:73:ALA:HB3	1.92	0.51
1:P:239:ARG:NH1	1:P:301:ALA:HB1	2.26	0.51
1:S:154:THR:HG23	1:S:156:LYS:HG2	1.93	0.51
1:S:95:GLU:HG3	1:S:98:ALA:HB2	1.92	0.51
2:U:24:ALA:HB1	2:U:27:TYR:CE1	2.45	0.51
1:B:7:ALA:O	1:B:11:THR:HG23	2.10	0.51
2:H:108:TYR:CB	3:L:51:GLY:HA3	2.41	0.51
1:R:85:ILE:HD11	1:R:112:ILE:HD11	1.92	0.51
2:W:161:VAL:HG22	2:W:206:VAL:HG22	1.92	0.51
1:D:183:LEU:HD21	1:D:186:THR:HG23	1.93	0.51
2:J:24:ALA:HB1	2:J:27:TYR:CE1	2.46	0.51
3:L:93:TRP:NE1	3:L:95:SER:HA	2.26	0.51
1:Q:19:ARG:HH11	1:Q:157:ASP:HA	1.76	0.51
1:Q:85:ILE:HD11	1:Q:112:ILE:HD11	1.93	0.51
1:T:154:THR:HG23	1:T:156:LYS:HG2	1.93	0.51
2:I:27:TYR:CE2	2:I:98:ARG:HD2	2.45	0.50
1:R:262:GLY:HA3	5:R:401:POV:H12	1.92	0.50
1:T:37:ARG:HH11	1:T:52:GLN:HE21	1.58	0.50
1:T:95:GLU:HG3	1:T:98:ALA:HB2	1.92	0.50
1:B:95:GLU:HG3	1:B:98:ALA:HB2	1.93	0.50
1:C:33:ASN:HB3	1:C:56:ARG:HB2	1.93	0.50
1:S:38:THR:HG22	1:S:52:GLN:HB3	1.92	0.50
2:U:98:ARG:NH2	2:U:110:ASP:OD2	2.36	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:170:GLN:NE2	3:N:172:ASN:OD1	2.45	0.50
1:T:38:THR:HG22	1:T:52:GLN:HB3	1.92	0.50
1:C:256:MET:HE3	1:C:283:CYS:HB3	1.94	0.50
2:I:132:PRO:HD3	2:I:217:LYS:HE2	1.93	0.50
2:Y:27:TYR:CE2	2:Y:98:ARG:HD2	2.46	0.50
1:T:126:LEU:HD13	1:T:128:LEU:HD21	1.92	0.50
2:U:133:LEU:HD23	2:U:150:LEU:HB2	1.92	0.50
1:C:154:THR:HG23	1:C:156:LYS:HG2	1.92	0.50
1:E:215:PHE:CE1	1:E:219:GLN:HG3	2.46	0.50
1:E:36:LEU:HD21	1:E:39:ILE:HD11	1.94	0.50
1:R:95:GLU:HG3	1:R:98:ALA:HB2	1.94	0.50
1:D:170:LEU:HD11	1:D:186:THR:HG21	1.94	0.50
1:P:10:PHE:HZ	1:P:85:ILE:HG22	1.77	0.50
1:R:137:TYR:O	1:R:275:ALA:HB3	2.12	0.50
1:S:19:ARG:HH11	1:S:157:ASP:HA	1.75	0.50
1:S:307:GLU:HG2	1:S:309:ASN:H	1.76	0.50
1:D:154:THR:HG22	1:D:155:THR:H	1.77	0.49
1:B:183:LEU:HD21	1:B:186:THR:HG23	1.93	0.49
1:S:194:VAL:O	2:X:55:ASN:ND2	2.43	0.49
2:V:162:THR:HG23	2:V:205:ASN:HB2	1.94	0.49
1:Q:126:LEU:HD13	1:Q:128:LEU:HD21	1.95	0.49
1:E:215:PHE:CZ	1:E:219:GLN:HG3	2.47	0.49
2:U:147:LEU:HD13	2:U:219:ILE:HD12	1.93	0.49
2:V:123:ALA:HB2	2:V:182:ASP:HB3	1.94	0.49
1:E:220:LEU:HD13	1:E:263:ILE:HG13	1.93	0.49
1:Q:138:PRO:HD2	1:Q:139:MET:SD	2.52	0.49
1:Q:95:GLU:HG3	1:Q:98:ALA:HB2	1.93	0.49
1:B:137:TYR:HD2	1:B:276:ILE:HB	1.77	0.49
3:N:37:TRP:CE2	3:N:75:LEU:HB2	2.46	0.49
1:R:284:MET:HG2	5:R:402:POV:H1	1.95	0.49
1:R:35:LEU:HB3	1:R:54:THR:HB	1.95	0.49
2:Y:60:TYR:HE1	2:Y:70:LEU:HG	1.78	0.49
1:D:217:LEU:O	1:D:221:TYR:HB2	2.12	0.49
1:S:134:LEU:N	1:S:272:TYR:OH	2.42	0.49
1:E:220:LEU:HD11	1:E:280:ILE:HD11	1.94	0.49
1:Q:154:THR:HG23	1:Q:156:LYS:HG2	1.93	0.49
1:P:271:SER:HB2	1:Q:180:SER:HA	1.95	0.49
1:A:154:THR:HG23	1:A:156:LYS:HG2	1.95	0.49
2:I:197:TRP:CZ3	2:I:202:VAL:HG22	2.48	0.49
3:M:37:TRP:CE2	3:M:75:LEU:HB2	2.48	0.49
1:T:141:VAL:HG11	1:T:208:GLN:HE21	1.78	0.49
1:C:170:LEU:HD11	1:C:186:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:27:TYR:CE2	2:J:98:ARG:HD2	2.47	0.48
1:P:170:LEU:HD11	1:P:186:THR:HG21	1.95	0.48
1:P:241:ALA:HB2	1:T:302:ASN:ND2	2.24	0.48
1:P:98:ALA:HB3	1:Q:103:ILE:HG21	1.95	0.48
1:Q:215:PHE:CE1	1:Q:219:GLN:HG3	2.48	0.48
1:D:126:LEU:HD13	1:D:128:LEU:HD21	1.95	0.48
1:E:19:ARG:HH11	1:E:157:ASP:HA	1.78	0.48
1:T:220:LEU:HB2	1:T:263:ILE:HD11	1.95	0.48
2:G:14:PRO:HG2	2:G:122:SER:HB3	1.95	0.48
1:S:111:ARG:HB2	1:S:119:LEU:HB3	1.94	0.48
2:Y:207:ALA:HB2	2:Y:214:LYS:HD3	1.95	0.48
1:C:224:SER:OG	1:C:283:CYS:SG	2.72	0.48
2:I:176:PRO:HG2	3:O:165:THR:HB	1.94	0.48
1:S:264:ASN:HD21	5:T:401:POV:H14B	1.78	0.48
3:Z:107:THR:HG21	3:Z:144:PRO:HB3	1.94	0.48
1:C:1:SER:HA	1:C:4:LYS:HD2	1.94	0.48
2:H:157:GLU:HG3	2:H:184:TYR:CD2	2.49	0.48
1:S:264:ASN:ND2	5:T:401:POV:H14B	2.28	0.48
3:L:148:THR:HB	3:L:199:THR:HB	1.94	0.48
3:N:170:GLN:NE2	3:N:174:LYS:HB2	2.29	0.48
1:R:138:PRO:HD2	1:R:139:MET:SD	2.53	0.48
1:C:111:ARG:HD2	1:C:119:LEU:HD23	1.94	0.48
2:U:6:GLN:N	2:U:114:GLN:HE22	2.12	0.48
1:B:134:LEU:N	1:B:272:TYR:OH	2.44	0.48
1:A:110:ILE:HG12	1:A:120:TYR:HD1	1.79	0.48
2:J:152:LYS:HA	2:J:185:THR:HG23	1.96	0.48
1:R:271:SER:HB2	1:S:180:SER:HA	1.96	0.48
1:C:288:PHE:HE1	1:D:230:VAL:HG11	1.78	0.47
3:L:85:GLU:HG3	3:L:107:THR:HA	1.96	0.47
1:P:220:LEU:O	1:P:224:SER:OG	2.23	0.47
1:T:311:ILE:O	1:T:315:VAL:HG23	2.14	0.47
1:C:271:SER:HB2	1:D:180:SER:HA	1.96	0.47
1:D:271:SER:HB2	1:E:180:SER:HA	1.95	0.47
2:W:168:LEU:HD13	2:W:190:VAL:HG21	1.96	0.47
1:B:300:ILE:O	1:B:308:TRP:HB3	2.13	0.47
2:J:24:ALA:HB1	2:J:27:TYR:HE1	1.77	0.47
1:A:170:LEU:HD22	1:A:174:LEU:HD23	1.96	0.47
1:D:285:THR:OG1	5:D:401:POV:O22	2.28	0.47
1:P:126:LEU:HD13	1:P:128:LEU:HD21	1.97	0.47
1:S:267:LEU:HG	1:S:268:PRO:O	2.15	0.47
2:G:157:GLU:HB2	2:G:158:PRO:HA	1.96	0.47
1:Q:259:GLN:O	1:Q:263:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:299:HIS:CE1	1:S:237:PHE:HA	2.49	0.47
1:Q:223:PRO:HB3	5:Q:401:POV:H3	1.97	0.47
1:S:85:ILE:HD11	1:S:112:ILE:HD11	1.97	0.47
1:B:220:LEU:O	1:B:224:SER:OG	2.21	0.47
1:C:230:VAL:O	1:C:233:VAL:HG22	2.14	0.47
2:H:6:GLN:N	2:H:114:GLN:HE22	2.12	0.47
1:Q:215:PHE:CZ	1:Q:219:GLN:HG3	2.49	0.47
1:S:137:TYR:HD2	1:S:276:ILE:HB	1.80	0.47
1:E:137:TYR:CE1	1:E:267:LEU:HD13	2.50	0.47
1:E:268:PRO:HA	1:E:269:PRO:HD3	1.77	0.47
2:G:161:VAL:HG22	2:G:206:VAL:HG22	1.96	0.47
2:G:44:ASN:ND2	3:K:102:GLY:HA2	2.30	0.47
2:X:155:PHE:HA	2:X:156:PRO:HA	1.76	0.47
3:M:120:LEU:HD13	3:M:209:LEU:HD22	1.97	0.47
1:R:230:VAL:O	1:R:233:VAL:HG22	2.14	0.47
1:R:220:LEU:HD22	1:R:263:ILE:HG13	1.96	0.47
1:T:170:LEU:HD11	1:T:186:THR:HG21	1.96	0.47
1:T:259:GLN:NE2	5:T:401:POV:O13	2.48	0.47
1:E:184:THR:CG2	1:E:210:LYS:HD2	2.45	0.47
2:F:175:PHE:CZ	3:N:138:THR:HG23	2.50	0.47
2:H:133:LEU:HD13	3:L:121:PHE:CG	2.50	0.47
1:Q:230:VAL:O	1:Q:233:VAL:HG22	2.14	0.47
1:S:185:ASN:HD22	4:S:401:NAG:H61	1.80	0.47
2:G:6:GLN:N	2:G:114:GLN:HE22	2.10	0.46
1:R:215:PHE:CZ	1:R:219:GLN:HG3	2.50	0.46
2:U:163:TRP:HB3	2:U:168:LEU:HD12	1.98	0.46
2:U:157:GLU:HG3	2:U:184:TYR:CD2	2.50	0.46
1:B:215:PHE:O	1:B:219:GLN:N	2.46	0.46
1:E:154:THR:HG23	1:E:156:LYS:HG2	1.95	0.46
2:G:208:HIS:CE1	2:G:211:SER:HG	2.30	0.46
1:R:227:LEU:HD13	5:R:401:POV:H34A	1.96	0.46
1:T:230:VAL:O	1:T:233:VAL:HG22	2.15	0.46
5:Q:401:POV:H13B	5:Q:401:POV:H11	1.64	0.46
1:E:175:SER:HB2	1:E:182:GLN:OE1	2.16	0.46
2:H:27:TYR:CE2	2:H:98:ARG:HD2	2.50	0.46
2:J:197:TRP:CZ2	2:J:221:PRO:HG3	2.50	0.46
2:G:208:HIS:NE2	2:G:210:ALA:HB3	2.31	0.46
1:Q:33:ASN:HB3	1:Q:56:ARG:HB2	1.98	0.46
1:R:297:VAL:HG13	1:R:312:SER:HB2	1.97	0.46
3:K:122:PRO:HG3	3:K:209:LEU:HD11	1.98	0.46
2:F:175:PHE:HZ	3:N:138:THR:HG23	1.81	0.46
2:Y:18:MET:HG3	2:Y:86:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Y:208:HIS:CE1	2:Y:210:ALA:HB3	2.51	0.46
1:A:170:LEU:HD11	1:A:186:THR:HG21	1.98	0.46
1:D:299:HIS:CE1	1:E:237:PHE:HA	2.51	0.46
3:K:151:TRP:O	3:K:157:PRO:HA	2.15	0.46
2:U:18:MET:HG3	2:U:86:LEU:HD11	1.97	0.46
1:B:299:HIS:CE1	1:C:237:PHE:HA	2.51	0.46
2:I:155:PHE:HA	2:I:156:PRO:HA	1.75	0.46
2:V:6:GLN:HE22	2:V:96:CYS:H	1.64	0.46
2:Y:174:THR:HG23	2:Y:186:LEU:HD21	1.97	0.46
1:C:35:LEU:HD12	1:C:169:GLN:O	2.16	0.46
1:T:137:TYR:HD2	1:T:276:ILE:HB	1.81	0.46
1:A:35:LEU:HB3	1:A:54:THR:HB	1.98	0.45
1:B:305:THR:CG2	1:B:308:TRP:HD1	2.28	0.45
2:G:37:VAL:HG11	2:G:45:LEU:HD23	1.98	0.45
1:C:19:ARG:HG2	1:C:20:PRO:HD2	1.98	0.45
2:F:132:PRO:HD3	2:F:217:LYS:HE2	1.97	0.45
2:H:132:PRO:HG3	2:H:217:LYS:HE2	1.97	0.45
2:I:108:TYR:CB	3:O:51:GLY:HA3	2.44	0.45
1:R:111:ARG:HB2	1:R:119:LEU:HB3	1.99	0.45
1:R:186:THR:HG22	1:R:207:ILE:HG22	1.98	0.45
1:S:271:SER:HB2	1:T:180:SER:HA	1.98	0.45
3:Z:22:CYS:HB3	3:Z:73:ALA:HB3	1.99	0.45
1:D:227:LEU:HG	1:D:252:THR:HG23	1.99	0.45
2:I:6:GLN:H	2:I:114:GLN:NE2	2.12	0.45
3:K:141:ASP:H	3:K:170:GLN:HE22	1.64	0.45
3:O:107:THR:HG21	3:O:144:PRO:HB3	1.99	0.45
1:S:170:LEU:HD22	1:S:174:LEU:HD23	1.99	0.45
2:V:6:GLN:N	2:V:114:GLN:HE22	2.11	0.45
2:H:127:PRO:HA	2:H:128:PRO:HD3	1.83	0.45
1:A:252:THR:HG22	1:A:287:ILE:HD13	1.98	0.45
1:B:130:CYS:O	1:B:132:MET:HG3	2.17	0.45
1:B:98:ALA:CB	1:C:103:ILE:HG13	2.46	0.45
1:E:183:LEU:HD12	1:E:183:LEU:O	2.17	0.45
2:F:6:GLN:N	2:F:114:GLN:HE22	2.14	0.45
2:H:50:LEU:HD21	2:H:59:SER:HB3	1.97	0.45
3:Z:150:ASP:O	3:Z:197:GLN:N	2.46	0.45
1:C:137:TYR:HA	1:C:138:PRO:HA	1.74	0.45
2:J:6:GLN:N	2:J:114:GLN:HE22	2.12	0.45
3:N:85:GLU:HG3	3:N:107:THR:HA	1.99	0.45
1:S:138:PRO:HD2	1:S:139:MET:SD	2.57	0.45
1:T:239:ARG:HD2	1:T:301:ALA:HB2	1.98	0.45
1:B:138:PRO:HG3	1:B:216:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:137:TYR:HA	1:D:138:PRO:HA	1.80	0.45
1:S:154:THR:HA	1:S:200:TYR:CD1	2.52	0.45
2:U:174:THR:HG23	2:U:186:LEU:HD21	1.98	0.45
2:V:141:THR:OG1	2:V:142:ASN:N	2.49	0.45
2:V:6:GLN:NE2	2:V:96:CYS:H	2.15	0.45
1:A:215:PHE:HA	1:E:273:ILE:HD11	1.99	0.45
1:C:239:ARG:HD2	1:C:301:ALA:HB1	1.98	0.45
1:D:20:PRO:HA	1:D:21:PRO:HD3	1.88	0.45
1:C:254:LEU:HD11	1:D:254:LEU:HD23	1.99	0.45
2:F:48:ILE:HA	2:F:64:PHE:HD2	1.81	0.45
1:R:215:PHE:CE1	1:R:219:GLN:HG3	2.52	0.45
1:A:230:VAL:O	1:A:233:VAL:HG22	2.17	0.45
1:C:138:PRO:HD2	1:C:139:MET:SD	2.57	0.45
1:E:259:GLN:O	1:E:263:ILE:HG12	2.17	0.45
1:B:137:TYR:HA	1:B:138:PRO:HA	1.69	0.45
1:B:230:VAL:O	1:B:233:VAL:HG22	2.16	0.45
2:G:176:PRO:HG2	3:K:165:THR:HB	1.98	0.45
1:C:313:LYS:HD3	1:C:313:LYS:HA	1.80	0.44
2:I:46:GLU:OE1	2:I:63:LYS:HE2	2.16	0.44
3:K:122:PRO:HB3	3:K:209:LEU:HD21	1.98	0.44
3:N:22:CYS:HB3	3:N:73:ALA:HB3	1.99	0.44
2:F:30:THR:HA	2:F:53:PRO:HB2	1.99	0.44
2:J:18:MET:HE2	2:J:18:MET:HB2	1.78	0.44
3:O:37:TRP:CE2	3:O:75:LEU:HB2	2.52	0.44
2:X:131:TYR:HA	2:X:132:PRO:HD3	1.83	0.44
1:E:267:LEU:HD12	1:E:268:PRO:HD2	1.99	0.44
1:P:239:ARG:HH11	1:P:301:ALA:HB1	1.81	0.44
1:S:259:GLN:O	1:S:263:ILE:HG12	2.18	0.44
2:U:199:SER:OG	2:U:200:GLU:OE1	2.28	0.44
2:V:163:TRP:HB2	2:V:168:LEU:HD11	1.99	0.44
2:H:146:THR:HG22	2:H:191:THR:HG22	2.00	0.44
2:J:20:ILE:HD13	2:J:81:MET:HE3	1.99	0.44
1:P:137:TYR:HA	1:P:138:PRO:HA	1.78	0.44
1:S:299:HIS:CE1	1:T:237:PHE:HA	2.52	0.44
1:A:107:ASN:OD1	1:A:123:ARG:NH1	2.50	0.44
3:K:109:LEU:HD21	3:K:144:PRO:HG3	2.00	0.44
1:Q:224:SER:HB2	1:Q:279:TRP:CZ3	2.53	0.44
1:R:267:LEU:HG	1:R:268:PRO:O	2.17	0.44
1:A:33:ASN:HB3	1:A:56:ARG:HB2	1.99	0.44
2:I:127:PRO:HA	2:I:128:PRO:HD3	1.83	0.44
2:J:60:TYR:HE1	2:J:70:LEU:HG	1.83	0.44
3:N:172:ASN:OD1	3:N:172:ASN:N	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:252:THR:HG22	1:R:287:ILE:HD13	2.00	0.44
1:R:305:THR:HG22	1:R:307:GLU:OE1	2.18	0.44
1:T:192:THR:O	2:Y:105:TYR:N	2.49	0.44
2:Y:6:GLN:N	2:Y:114:GLN:HE22	2.12	0.44
1:E:49:TYR:CE1	1:E:144:CYS:HB3	2.52	0.44
2:J:208:HIS:CE1	2:J:210:ALA:HB3	2.53	0.44
5:P:403:POV:H13B	5:P:403:POV:H11A	1.77	0.44
1:Q:311:ILE:O	1:Q:315:VAL:HG23	2.18	0.44
1:S:33:ASN:HB3	1:S:56:ARG:HB2	2.00	0.44
2:X:208:HIS:CE1	2:X:210:ALA:HB3	2.53	0.44
1:A:310:ASP:O	1:A:314:ARG:HG3	2.18	0.44
1:D:175:SER:HB2	1:D:182:GLN:OE1	2.18	0.44
1:D:194:VAL:HG13	2:I:52:ASN:HD22	1.82	0.44
1:C:194:VAL:HG13	2:G:52:ASN:HD22	1.82	0.44
2:G:6:GLN:H	2:G:114:GLN:NE2	2.13	0.44
2:G:153:GLY:HA2	2:G:183:LEU:HD22	2.00	0.44
3:L:37:TRP:CZ3	3:L:90:CYS:HB3	2.53	0.44
1:P:68:VAL:N	1:P:71:ASP:OD2	2.49	0.44
1:Q:111:ARG:HB2	1:Q:119:LEU:HB3	1.99	0.44
1:R:96:LYS:HD2	1:R:129:SER:HB3	2.00	0.44
2:W:157:GLU:HG3	2:W:184:TYR:CD2	2.53	0.44
2:W:60:TYR:CE1	2:W:70:LEU:HG	2.53	0.44
2:Y:144:MET:HG2	2:Y:193:PRO:HA	2.00	0.44
1:A:299:HIS:CE1	1:B:237:PHE:HA	2.53	0.43
1:C:19:ARG:HH11	1:C:157:ASP:HA	1.82	0.43
2:J:177:ALA:HB2	2:J:186:LEU:HD23	2.00	0.43
3:M:152:LYS:HB2	3:M:195:SER:HB3	1.99	0.43
3:O:37:TRP:CZ3	3:O:90:CYS:HB3	2.53	0.43
1:R:311:ILE:O	1:R:315:VAL:HG23	2.18	0.43
1:S:309:ASN:OD1	1:S:311:ILE:HG12	2.18	0.43
1:E:230:VAL:O	1:E:233:VAL:HG22	2.18	0.43
1:T:137:TYR:O	1:T:275:ALA:HB3	2.18	0.43
2:W:6:GLN:N	2:W:114:GLN:HE22	2.11	0.43
2:W:208:HIS:CE1	2:W:210:ALA:HB3	2.53	0.43
2:H:153:GLY:HA2	2:H:183:LEU:HB3	1.99	0.43
3:M:41:LYS:HE2	3:M:83:GLU:O	2.18	0.43
1:S:100:LYS:HE2	1:T:104:ASP:H	1.83	0.43
1:A:300:ILE:HG13	1:A:312:SER:OG	2.18	0.43
1:D:252:THR:HG22	1:D:287:ILE:HD13	2.00	0.43
1:P:230:VAL:O	1:P:233:VAL:HG22	2.18	0.43
1:R:220:LEU:HD23	1:R:276:ILE:HD11	2.01	0.43
1:S:224:SER:HB2	1:S:279:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:48:ILE:HG12	2:F:64:PHE:CE2	2.54	0.43
3:N:199:THR:HA	3:N:204:THR:HA	2.01	0.43
2:F:108:TYR:HB3	3:N:52:GLY:H	1.84	0.43
1:P:259:GLN:HE22	5:P:403:POV:P	2.42	0.43
1:P:305:THR:HB	1:P:308:TRP:HD1	1.83	0.43
1:R:249:GLY:HA3	1:R:291:LEU:HD13	1.99	0.43
1:S:170:LEU:HD11	1:S:186:THR:HG21	2.01	0.43
1:S:183:LEU:HD11	1:S:207:ILE:HB	2.01	0.43
8:T:403:LMT:H5B	8:T:403:LMT:H6D	2.01	0.43
1:C:311:ILE:O	1:C:315:VAL:HG23	2.19	0.43
2:I:161:VAL:HG22	2:I:206:VAL:HG22	1.99	0.43
3:K:188:TRP:CG	3:K:189:GLU:N	2.87	0.43
3:L:41:LYS:HB2	3:L:45:LEU:HB2	1.99	0.43
1:A:19:ARG:HH11	1:A:157:ASP:HA	1.83	0.43
2:H:164:ASN:HB3	2:H:167:SER:HB3	1.99	0.43
1:P:137:TYR:O	1:P:275:ALA:HB3	2.18	0.43
2:U:27:TYR:CE2	2:U:98:ARG:HD2	2.53	0.43
1:A:220:LEU:HD23	1:A:276:ILE:HD11	2.01	0.43
2:F:108:TYR:CB	3:N:51:GLY:HA2	2.49	0.43
1:Q:183:LEU:O	1:Q:183:LEU:HD12	2.19	0.43
1:Q:267:LEU:HA	1:Q:268:PRO:HD2	1.87	0.43
1:S:222:ILE:HB	1:S:223:PRO:HD3	2.00	0.43
3:K:85:GLU:HG3	3:K:107:THR:HA	1.99	0.43
1:P:138:PRO:HD2	1:P:139:MET:SD	2.59	0.43
1:R:137:TYR:HA	1:R:138:PRO:HA	1.79	0.43
1:S:220:LEU:C	1:S:223:PRO:HD2	2.38	0.43
1:S:49:TYR:CE1	1:S:144:CYS:HB3	2.54	0.43
1:B:111:ARG:HD2	1:B:119:LEU:HD23	2.00	0.43
1:B:267:LEU:HD12	1:B:268:PRO:HD2	2.00	0.43
2:F:133:LEU:HD13	3:N:121:PHE:CG	2.53	0.43
3:L:139:ILE:HD12	3:L:198:VAL:HG21	2.00	0.43
1:R:20:PRO:HA	1:R:21:PRO:HD3	1.86	0.43
2:U:135:PRO:HB2	2:U:140:GLN:HE22	1.84	0.43
2:X:18:MET:HG3	2:X:86:LEU:HD11	2.00	0.43
1:B:215:PHE:CZ	1:B:219:GLN:HG2	2.54	0.42
1:B:20:PRO:HA	1:B:21:PRO:HD3	1.86	0.42
1:D:138:PRO:HD2	1:D:139:MET:SD	2.59	0.42
1:D:267:LEU:HA	1:D:268:PRO:HD2	1.92	0.42
2:G:144:MET:HB2	2:G:191:THR:HG22	2.01	0.42
3:O:45:LEU:HD13	3:O:45:LEU:HA	1.87	0.42
1:Q:134:LEU:HD12	1:Q:270:VAL:HG21	2.00	0.42
1:R:300:ILE:HB	1:R:308:TRP:HE3	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:U:208:HIS:CE1	2:U:210:ALA:HB3	2.54	0.42
1:A:136:TYR:O	1:A:140:ASP:HB3	2.19	0.42
1:A:138:PRO:HD2	1:A:139:MET:SD	2.59	0.42
1:B:10:PHE:HE2	1:B:83:HIS:HB3	1.80	0.42
1:B:267:LEU:HA	1:B:268:PRO:HD2	1.90	0.42
2:F:127:PRO:HA	2:F:128:PRO:HD3	1.85	0.42
3:M:122:PRO:HG3	3:M:209:LEU:HD11	2.00	0.42
1:R:33:ASN:HB3	1:R:56:ARG:HB2	2.00	0.42
1:C:299:HIS:CE1	1:D:237:PHE:HA	2.54	0.42
1:R:19:ARG:HH11	1:R:157:ASP:HA	1.84	0.42
1:B:170:LEU:HD11	1:B:186:THR:HG21	2.01	0.42
1:D:313:LYS:HA	1:D:313:LYS:HD3	1.88	0.42
1:P:311:ILE:O	1:P:315:VAL:HG23	2.19	0.42
1:B:227:LEU:HG	1:B:252:THR:HG23	2.01	0.42
1:C:114:ASN:N	1:C:114:ASN:OD1	2.53	0.42
1:D:224:SER:HB2	1:D:279:TRP:CZ3	2.55	0.42
1:P:20:PRO:HA	1:P:21:PRO:HD3	1.88	0.42
1:R:189:THR:OG1	1:R:190:TYR:N	2.52	0.42
5:R:402:POV:H28A	5:R:402:POV:H211	1.73	0.42
1:C:130:CYS:O	1:C:132:MET:HG3	2.20	0.42
1:B:220:LEU:HD23	1:B:276:ILE:HD11	2.01	0.42
1:C:217:LEU:HA	1:C:221:TYR:HB2	2.01	0.42
1:C:267:LEU:HD12	1:C:268:PRO:HD2	2.02	0.42
3:K:141:ASP:H	3:K:170:GLN:NE2	2.18	0.42
3:N:118:VAL:O	3:N:207:LYS:HE3	2.20	0.42
1:S:300:ILE:HD11	1:S:312:SER:HA	2.02	0.42
1:T:224:SER:HB2	1:T:279:TRP:CZ3	2.55	0.42
2:X:33:THR:HA	2:X:53:PRO:HD3	2.00	0.42
1:A:76:PHE:CD2	1:A:111:ARG:HD3	2.55	0.42
1:C:8:HIS:O	1:C:11:THR:HG22	2.19	0.42
1:B:273:ILE:HD11	1:C:215:PHE:HA	2.02	0.42
1:D:76:PHE:CD2	1:D:111:ARG:HD3	2.55	0.42
1:D:168:LEU:HD23	1:D:186:THR:HB	2.01	0.42
1:D:227:LEU:HD12	1:D:227:LEU:HA	1.88	0.42
2:I:133:LEU:HD13	3:O:121:PHE:CG	2.55	0.42
1:P:252:THR:HG22	1:P:287:ILE:HD13	2.01	0.42
1:S:114:ASN:N	1:S:114:ASN:OD1	2.53	0.42
1:T:138:PRO:HD2	1:T:139:MET:SD	2.59	0.42
1:T:261:ALA:O	1:T:264:ASN:HB2	2.20	0.42
1:D:215:PHE:CE1	1:D:219:GLN:HG3	2.55	0.42
1:E:267:LEU:HA	1:E:268:PRO:HD2	1.81	0.42
2:J:18:MET:HG3	2:J:86:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:221:TYR:HA	1:C:279:TRP:CZ3	2.55	0.42
2:F:178:VAL:HG12	2:F:180:GLN:H	1.85	0.42
2:F:48:ILE:HA	2:F:64:PHE:CD2	2.55	0.42
3:K:129:GLU:O	3:K:130:THR:OG1	2.34	0.42
2:I:61:ASN:HD21	3:O:97:HIS:HE1	1.66	0.42
1:P:111:ARG:HD2	1:P:119:LEU:HD23	2.01	0.42
1:S:75:ASP:O	1:S:114:ASN:N	2.53	0.42
2:V:155:PHE:HA	2:V:156:PRO:HA	1.76	0.42
2:W:18:MET:HE1	2:W:20:ILE:HG12	2.01	0.42
2:X:170:SER:OG	2:X:171:GLY:N	2.52	0.42
1:S:194:VAL:HG13	2:X:52:ASN:HD22	1.85	0.42
1:B:102:THR:HA	1:B:106:PRO:HA	2.02	0.41
1:C:134:LEU:HD12	1:C:270:VAL:HG21	2.01	0.41
1:C:137:TYR:O	1:C:275:ALA:HB3	2.20	0.41
2:F:144:MET:HG2	2:F:193:PRO:HA	2.02	0.41
2:J:53:PRO:O	2:J:74:LYS:HE2	2.20	0.41
3:L:94:TYR:O	3:L:95:SER:OG	2.29	0.41
2:W:18:MET:HG3	2:W:86:LEU:HD11	2.01	0.41
1:B:189:THR:OG1	1:B:190:TYR:N	2.53	0.41
1:D:138:PRO:HB2	1:D:211:ARG:HD2	2.02	0.41
3:N:152:LYS:HD3	3:N:197:GLN:OE1	2.20	0.41
1:Q:130:CYS:HA	1:Q:131:PRO:HD2	1.95	0.41
1:R:130:CYS:O	1:R:132:MET:HG3	2.19	0.41
2:V:157:GLU:HG3	2:V:184:TYR:CD2	2.56	0.41
1:C:111:ARG:HB2	1:C:119:LEU:HB3	2.00	0.41
1:E:19:ARG:HG2	1:E:20:PRO:HD2	2.02	0.41
2:F:155:PHE:HA	2:F:156:PRO:HA	1.76	0.41
1:T:307:GLU:O	1:T:311:ILE:HG12	2.19	0.41
2:U:100:GLY:HA3	2:U:108:TYR:CZ	2.55	0.41
2:H:208:HIS:NE2	2:H:210:ALA:HB3	2.34	0.41
3:K:94:TYR:O	3:K:96:ASN:N	2.53	0.41
1:C:273:ILE:HG12	1:D:215:PHE:HD1	1.85	0.41
1:P:279:TRP:HB2	1:P:334:TYR:CE1	2.56	0.41
1:Q:76:PHE:CD2	1:Q:111:ARG:HD3	2.56	0.41
1:S:154:THR:HA	1:S:200:TYR:HD1	1.85	0.41
3:Z:181:LEU:HG	3:Z:183:LEU:HD13	2.01	0.41
1:A:237:PHE:HA	1:E:299:HIS:CE1	2.55	0.41
2:G:18:MET:HG3	2:G:86:LEU:HD11	2.01	0.41
1:P:288:PHE:CG	5:Q:401:POV:H34	2.56	0.41
2:U:197:TRP:HA	2:U:198:PRO:HA	1.86	0.41
1:A:137:TYR:CE2	1:A:138:PRO:HB3	2.56	0.41
1:B:19:ARG:HG2	1:B:20:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:262:GLY:HA2	5:R:401:POV:H14B	2.03	0.41
3:Z:166:GLN:HA	3:Z:167:PRO:HD2	1.91	0.41
1:A:271:SER:HB2	1:B:180:SER:HA	2.03	0.41
3:K:121:PHE:HA	3:K:122:PRO:HD3	1.80	0.41
3:L:187:ALA:O	3:L:191:HIS:ND1	2.51	0.41
2:V:166:GLY:C	2:V:168:LEU:H	2.24	0.41
3:Z:115:SER:HA	3:Z:116:PRO:HD3	1.92	0.41
1:B:20:PRO:HD3	1:B:86:TRP:CD2	2.56	0.41
1:E:130:CYS:O	1:E:132:MET:HG3	2.20	0.41
1:E:170:LEU:HD22	1:E:174:LEU:HD23	2.01	0.41
1:E:20:PRO:HA	1:E:21:PRO:HD3	1.85	0.41
1:P:130:CYS:O	1:P:132:MET:HG3	2.21	0.41
2:Y:169:SER:C	2:Y:171:GLY:H	2.24	0.41
2:Y:153:GLY:HA2	2:Y:183:LEU:HB3	2.03	0.41
2:Y:27:TYR:HD2	2:Y:32:TYR:CD1	2.39	0.41
1:B:19:ARG:HH11	1:B:157:ASP:HA	1.86	0.41
1:E:227:LEU:HD12	1:E:227:LEU:HA	1.89	0.41
1:E:279:TRP:HB2	1:E:334:TYR:CZ	2.56	0.41
1:E:35:LEU:HB3	1:E:54:THR:HB	2.03	0.41
2:H:6:GLN:H	2:H:114:GLN:NE2	2.17	0.41
2:J:177:ALA:HA	2:J:186:LEU:HB3	2.02	0.41
3:L:128:LEU:HD21	3:L:188:TRP:CZ3	2.55	0.41
3:M:40:GLU:O	3:M:86:ALA:HB1	2.20	0.41
1:R:49:TYR:CE1	1:R:144:CYS:HB3	2.56	0.41
1:T:130:CYS:O	1:T:132:MET:HG3	2.21	0.41
2:W:121:SER:OG	2:W:182:ASP:OD1	2.39	0.41
2:Y:13:ARG:HD2	2:Y:122:SER:HA	2.03	0.41
3:Z:188:TRP:HA	3:Z:194:TYR:OH	2.20	0.41
2:J:218:LYS:HG2	2:J:219:ILE:H	1.86	0.41
1:T:220:LEU:HD23	1:T:276:ILE:HD11	2.02	0.41
2:U:18:MET:HE1	2:U:20:ILE:HG12	2.02	0.41
2:Y:131:TYR:HA	2:Y:132:PRO:HD3	1.87	0.41
1:A:137:TYR:HA	1:A:138:PRO:HA	1.79	0.40
1:A:35:LEU:HD12	1:A:169:GLN:O	2.21	0.40
1:B:43:ASP:OD1	1:B:45:VAL:N	2.51	0.40
1:Q:96:LYS:HD2	1:Q:129:SER:HB3	2.03	0.40
1:E:110:ILE:HG12	1:E:120:TYR:HD1	1.85	0.40
2:I:33:THR:HA	2:I:53:PRO:HD3	2.03	0.40
1:Q:107:ASN:OD1	1:Q:123:ARG:NH1	2.54	0.40
1:C:49:TYR:CE1	1:C:144:CYS:HB3	2.56	0.40
2:H:155:PHE:HA	2:H:156:PRO:HA	1.80	0.40
3:L:188:TRP:HA	3:L:194:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:53:ILE:CG2	3:N:54:ASN:N	2.84	0.40
1:P:19:ARG:HA	1:P:20:PRO:HD3	1.97	0.40
1:S:302:ASN:ND2	1:T:241:ALA:HA	2.36	0.40
1:S:5:ILE:O	1:S:8:HIS:HB3	2.20	0.40
1:T:183:LEU:O	1:T:183:LEU:HD12	2.22	0.40
1:T:35:LEU:HD12	1:T:169:GLN:O	2.22	0.40
2:V:179:LEU:HD12	2:V:184:TYR:HE1	1.87	0.40
2:W:147:LEU:HD22	2:W:219:ILE:HG21	2.03	0.40
2:X:6:GLN:N	2:X:114:GLN:HE22	2.20	0.40
1:A:19:ARG:HG2	1:A:20:PRO:HD2	2.04	0.40
1:C:220:LEU:HD23	1:C:276:ILE:HD11	2.02	0.40
1:E:134:LEU:N	1:E:272:TYR:OH	2.41	0.40
2:H:18:MET:HG3	2:H:86:LEU:HD11	2.04	0.40
1:S:19:ARG:HG2	1:S:20:PRO:HD2	2.04	0.40
1:T:300:ILE:HG23	1:T:308:TRP:CE3	2.49	0.40
2:X:126:THR:HA	2:X:127:PRO:HD3	1.96	0.40
1:A:267:LEU:HD22	1:A:276:ILE:HG21	2.04	0.40
2:F:152:LYS:HA	2:F:185:THR:HG23	2.04	0.40
2:H:134:ALA:HA	2:H:135:PRO:HD3	1.97	0.40
2:I:48:ILE:HA	2:I:64:PHE:CD2	2.57	0.40
3:K:148:THR:HB	3:K:199:THR:HB	2.03	0.40
1:S:19:ARG:NH1	1:S:157:ASP:HA	2.37	0.40
1:S:137:TYR:OH	1:S:267:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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	340/347 (98%)	327 (96%)	13 (4%)	0	100	100
1	B	339/347 (98%)	325 (96%)	14 (4%)	0	100	100
1	C	338/347 (97%)	324 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	338/347 (97%)	328 (97%)	10 (3%)	0	100	100
1	E	338/347 (97%)	325 (96%)	13 (4%)	0	100	100
1	P	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
1	Q	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
1	R	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
1	S	338/347 (97%)	325 (96%)	12 (4%)	1 (0%)	50	91
1	T	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
2	F	219/224 (98%)	206 (94%)	13 (6%)	0	100	100
2	G	220/224 (98%)	203 (92%)	17 (8%)	0	100	100
2	H	221/224 (99%)	206 (93%)	15 (7%)	0	100	100
2	I	220/224 (98%)	206 (94%)	14 (6%)	0	100	100
2	J	220/224 (98%)	203 (92%)	16 (7%)	1 (0%)	38	85
2	U	219/224 (98%)	205 (94%)	14 (6%)	0	100	100
2	V	222/224 (99%)	203 (91%)	19 (9%)	0	100	100
2	W	222/224 (99%)	209 (94%)	13 (6%)	0	100	100
2	X	222/224 (99%)	206 (93%)	16 (7%)	0	100	100
2	Y	219/224 (98%)	202 (92%)	17 (8%)	0	100	100
3	K	208/215 (97%)	193 (93%)	14 (7%)	1 (0%)	38	85
3	L	209/215 (97%)	198 (95%)	11 (5%)	0	100	100
3	M	208/215 (97%)	193 (93%)	15 (7%)	0	100	100
3	N	209/215 (97%)	194 (93%)	14 (7%)	1 (0%)	38	85
3	O	209/215 (97%)	194 (93%)	15 (7%)	0	100	100
3	Z	213/215 (99%)	193 (91%)	19 (9%)	1 (0%)	38	85
3	f	213/215 (99%)	195 (92%)	16 (8%)	2 (1%)	25	76
3	g	209/215 (97%)	196 (94%)	11 (5%)	2 (1%)	22	74
3	h	209/215 (97%)	194 (93%)	15 (7%)	0	100	100
3	i	212/215 (99%)	199 (94%)	12 (6%)	1 (0%)	38	85
All	All	7686/7860 (98%)	7256 (94%)	420 (6%)	10 (0%)	59	95

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	95	SER

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Mol	Chain	Res	Type
3	N	95	SER
3	i	95	SER
3	f	95	SER
1	S	309	ASN
3	f	96	ASN
2	J	221	PRO
3	g	96	ASN
3	g	52	GLY
3	Z	52	GLY

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	311/316 (98%)	310 (100%)	1 (0%)	96 99
1	B	310/316 (98%)	310 (100%)	0	100 100
1	C	309/316 (98%)	309 (100%)	0	100 100
1	D	309/316 (98%)	307 (99%)	2 (1%)	92 98
1	E	309/316 (98%)	309 (100%)	0	100 100
1	P	309/316 (98%)	308 (100%)	1 (0%)	96 99
1	Q	309/316 (98%)	308 (100%)	1 (0%)	96 99
1	R	309/316 (98%)	309 (100%)	0	100 100
1	S	309/316 (98%)	309 (100%)	0	100 100
1	T	309/316 (98%)	309 (100%)	0	100 100
2	F	190/193 (98%)	189 (100%)	1 (0%)	94 98
2	G	191/193 (99%)	190 (100%)	1 (0%)	94 98
2	H	192/193 (100%)	191 (100%)	1 (0%)	94 98
2	I	191/193 (99%)	190 (100%)	1 (0%)	94 98
2	J	191/193 (99%)	190 (100%)	1 (0%)	94 98
2	U	190/193 (98%)	188 (99%)	2 (1%)	84 96
2	V	193/193 (100%)	192 (100%)	1 (0%)	94 98
2	W	193/193 (100%)	193 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	X	193/193 (100%)	192 (100%)	1 (0%)	94 98
2	Y	190/193 (98%)	188 (99%)	2 (1%)	84 96
3	K	178/182 (98%)	178 (100%)	0	100 100
3	L	179/182 (98%)	179 (100%)	0	100 100
3	M	178/182 (98%)	177 (99%)	1 (1%)	92 98
3	N	179/182 (98%)	179 (100%)	0	100 100
3	O	179/182 (98%)	177 (99%)	2 (1%)	84 96
3	Z	182/182 (100%)	181 (100%)	1 (0%)	94 98
3	f	182/182 (100%)	181 (100%)	1 (0%)	94 98
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%)	179 (99%)	2 (1%)	84 96
All	All	6803/6910 (98%)	6780 (100%)	23 (0%)	96 99

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	LEU
1	D	154	THR
1	D	264	ASN
2	F	27	TYR
2	G	220	VAL
2	H	27	TYR
2	I	27	TYR
3	O	96	ASN
3	O	97	HIS
1	P	105	LYS
1	Q	264	ASN
2	U	27	TYR
2	U	196	THR
2	V	149	CYS
2	X	45	LEU
2	Y	27	TYR
2	Y	45	LEU
3	Z	56	ARG
3	f	96	ASN
3	i	97	HIS
3	i	214	CYS

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Mol	Chain	Res	Type
2	J	27	TYR
3	M	130	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	219	GLN
1	E	259	GLN
2	H	140	GLN
3	K	170	GLN
3	L	200	HIS
3	N	170	GLN
3	O	97	HIS
1	P	73	GLN
1	Q	299	HIS
1	S	264	ASN
3	Z	97	HIS
3	f	39	GLN
3	h	39	GLN
3	h	170	GLN

5.3.3 RNA

There are no RNA chains 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

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	12,14,15	0.53	0	15,19,21	0.94	1 (6%)
5	POV	A	402	-	22,22,51	1.63	2 (9%)	29,29,59	1.25	3 (10%)
7	GOL	B	401	-	5,5,5	0.34	0	5,5,5	0.24	0
4	NAG	B	402	1	12,14,15	0.51	0	15,19,21	0.82	1 (6%)
8	LMT	B	403	-	24,24,36	1.30	3 (12%)	34,35,47	1.56	6 (17%)
4	NAG	C	401	1	12,14,15	0.72	1 (8%)	15,19,21	0.74	0
8	LMT	C	402	-	24,24,36	1.37	3 (12%)	34,35,47	1.16	2 (5%)
5	POV	D	401	-	25,25,51	2.16	4 (16%)	33,33,59	1.28	3 (9%)
4	NAG	D	402	1	12,14,15	0.51	0	15,19,21	1.34	1 (6%)
8	LMT	D	403	-	24,24,36	1.35	3 (12%)	34,35,47	1.23	3 (8%)
4	NAG	E	401	1	12,14,15	0.49	0	15,19,21	0.78	1 (6%)
8	LMT	E	402	-	24,24,36	1.32	3 (12%)	34,35,47	1.17	3 (8%)
4	NAG	P	401	1	12,14,15	0.49	0	15,19,21	1.04	1 (6%)
8	LMT	P	402	-	24,24,36	1.32	3 (12%)	34,35,47	1.25	3 (8%)
5	POV	P	403	-	41,41,51	1.37	3 (7%)	49,49,59	1.06	4 (8%)
5	POV	Q	401	-	45,45,51	1.33	3 (6%)	53,53,59	1.01	3 (5%)
4	NAG	Q	402	1	12,14,15	0.46	0	15,19,21	0.79	0
5	POV	R	401	-	33,33,51	1.85	4 (12%)	41,41,59	1.08	3 (7%)
5	POV	R	402	-	34,34,51	2.02	5 (14%)	39,39,59	1.44	6 (15%)
4	NAG	S	401	1	12,14,15	0.45	0	15,19,21	1.20	3 (20%)
8	LMT	S	402	-	24,24,36	1.33	3 (12%)	34,35,47	1.26	3 (8%)
5	POV	T	401	-	41,42,51	1.03	2 (4%)	49,50,59	1.10	4 (8%)
4	NAG	T	402	1	12,14,15	0.53	0	15,19,21	0.96	1 (6%)
8	LMT	T	403	-	24,24,36	1.33	3 (12%)	34,35,47	1.29	5 (14%)

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	POV	A	402	-	-	0/25/25/55	0/0/0/0
7	GOL	B	401	-	-	0/4/4/4	0/0/0/0
4	NAG	B	402	1	-	0/6/23/26	0/1/1/1
8	LMT	B	403	-	-	0/8/48/61	0/2/2/2
4	NAG	C	401	1	-	0/6/23/26	0/1/1/1
8	LMT	C	402	-	-	0/8/48/61	0/2/2/2
5	POV	D	401	-	-	0/29/29/55	0/0/0/0
4	NAG	D	402	1	-	0/6/23/26	0/1/1/1
8	LMT	D	403	-	-	0/8/48/61	0/2/2/2
4	NAG	E	401	1	-	0/6/23/26	0/1/1/1
8	LMT	E	402	-	-	0/8/48/61	0/2/2/2
4	NAG	P	401	1	-	0/6/23/26	0/1/1/1
8	LMT	P	402	-	-	0/8/48/61	0/2/2/2
5	POV	P	403	-	-	0/45/45/55	0/0/0/0
5	POV	Q	401	-	-	0/49/49/55	0/0/0/0
4	NAG	Q	402	1	-	0/6/23/26	0/1/1/1
5	POV	R	401	-	-	1/37/37/55	0/0/0/0
5	POV	R	402	-	-	0/36/36/55	0/0/0/0
4	NAG	S	401	1	-	0/6/23/26	0/1/1/1
8	LMT	S	402	-	-	0/8/48/61	0/2/2/2
5	POV	T	401	-	-	0/46/46/55	0/0/0/0
4	NAG	T	402	1	-	1/6/23/26	0/1/1/1
8	LMT	T	403	-	-	0/8/48/61	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	POV	C24-C23	-6.15	1.52	1.55
5	R	402	POV	C37-C36	-6.12	1.52	1.55
5	R	401	POV	C310-C39	-6.07	1.52	1.55
5	Q	401	POV	C310-C39	-5.95	1.52	1.55
5	D	401	POV	C34-C33	-5.93	1.52	1.55
5	P	403	POV	C28-C27	-5.82	1.52	1.55
5	R	401	POV	C26-C25	-5.76	1.52	1.55
5	A	402	POV	C26-C25	-5.74	1.52	1.55
5	R	402	POV	C216-C215	-5.74	1.52	1.55
5	R	402	POV	P-O12	5.71	1.61	1.51
5	D	401	POV	O31-C31	4.28	1.46	1.33
5	P	403	POV	O31-C31	4.16	1.46	1.33
5	Q	401	POV	O31-C31	4.14	1.46	1.33
5	R	401	POV	O31-C31	4.08	1.45	1.33
5	T	401	POV	O31-C31	4.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	402	POV	O31-C31	4.02	1.45	1.33
5	R	402	POV	O21-C21	3.88	1.46	1.34
5	A	402	POV	O21-C21	3.85	1.45	1.34
5	Q	401	POV	O21-C21	3.80	1.45	1.34
5	T	401	POV	O21-C21	3.80	1.45	1.34
5	P	403	POV	O21-C21	3.79	1.45	1.34
5	R	401	POV	O21-C21	3.77	1.45	1.34
5	D	401	POV	O21-C21	3.69	1.45	1.34
8	T	403	LMT	O1'-C1'	3.46	1.40	1.23
8	D	403	LMT	O1'-C1'	3.44	1.40	1.23
8	P	402	LMT	O1'-C1'	3.43	1.40	1.23
8	B	403	LMT	O1'-C1'	3.42	1.40	1.23
8	E	402	LMT	O1'-C1'	3.41	1.40	1.23
8	S	402	LMT	O1'-C1'	3.41	1.40	1.23
8	C	402	LMT	O1'-C1'	3.40	1.40	1.23
8	S	402	LMT	O5'-C1'	3.14	1.48	1.41
8	T	403	LMT	O5'-C1'	3.12	1.48	1.41
8	C	402	LMT	O5'-C1'	3.11	1.48	1.41
8	P	402	LMT	O5'-C1'	3.02	1.48	1.41
8	C	402	LMT	O5B-C1B	3.01	1.49	1.41
8	D	403	LMT	O5B-C1B	2.97	1.49	1.41
8	D	403	LMT	O5'-C1'	2.96	1.48	1.41
8	E	402	LMT	O5'-C1'	2.91	1.48	1.41
8	B	403	LMT	O5B-C1B	2.88	1.49	1.41
8	P	402	LMT	O5B-C1B	2.85	1.49	1.41
8	B	403	LMT	O5'-C1'	2.79	1.47	1.41
8	S	402	LMT	O5B-C1B	2.71	1.48	1.41
8	T	403	LMT	O5B-C1B	2.66	1.48	1.41
8	E	402	LMT	O5B-C1B	2.58	1.48	1.41
4	C	401	NAG	O5-C5	-2.15	1.42	1.45

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	402	POV	O21-C21-C22	4.34	120.79	111.54
5	T	401	POV	O21-C21-C22	4.22	120.53	111.54
8	B	403	LMT	C1'-C2'-C3'	4.13	115.93	109.11
4	D	402	NAG	O5-C5-C6	4.12	111.30	106.98
5	A	402	POV	O21-C21-C22	4.10	120.28	111.54
5	D	401	POV	O21-C21-C22	4.08	120.23	111.54
5	P	403	POV	O21-C21-C22	3.86	119.76	111.54
8	E	402	LMT	O5'-C5'-C4'	3.63	117.32	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	401	POV	C2-O21-C21	-3.46	109.72	117.86
4	P	401	NAG	O5-C5-C6	3.44	110.59	106.98
5	R	401	POV	C2-O21-C21	-3.43	109.79	117.86
8	S	402	LMT	C1B-O1B-C4'	-3.37	109.45	118.00
8	P	402	LMT	C1B-O1B-C4'	-3.34	109.52	118.00
5	R	401	POV	O21-C21-C22	3.29	118.55	111.54
5	Q	401	POV	O21-C21-C22	3.28	118.53	111.54
8	D	403	LMT	C1'-C2'-C3'	3.25	114.48	109.11
8	P	402	LMT	C1'-C2'-C3'	3.19	114.37	109.11
4	A	401	NAG	O5-C5-C6	3.04	110.17	106.98
5	P	403	POV	C2-O21-C21	-3.02	110.75	117.86
5	Q	401	POV	O31-C31-C32	3.02	121.15	111.90
8	T	403	LMT	C1'-C2'-C3'	3.02	114.09	109.11
5	R	402	POV	O13-P-O14	3.01	119.72	112.74
8	B	403	LMT	C2'-C3'-C4'	2.94	115.97	109.59
5	T	401	POV	C2-O21-C21	-2.92	110.99	117.86
5	A	402	POV	O31-C3-C2	-2.92	109.21	113.35
8	T	403	LMT	C1B-O1B-C4'	-2.87	110.71	118.00
5	R	401	POV	O31-C31-C32	2.76	120.35	111.90
5	R	402	POV	O31-C31-C32	2.73	120.25	111.90
5	D	401	POV	O31-C31-C32	2.72	120.21	111.90
8	P	402	LMT	C2'-C3'-C4'	2.66	115.37	109.59
5	R	402	POV	C2-O21-C21	-2.65	111.62	117.86
8	B	403	LMT	O5B-C5B-C4B	2.65	114.65	109.73
8	D	403	LMT	C1B-O1B-C4'	-2.62	111.35	118.00
5	P	403	POV	O31-C31-C32	2.61	119.89	111.90
5	A	402	POV	C2-O21-C21	-2.60	111.75	117.86
4	S	401	NAG	O5-C5-C6	2.60	109.71	106.98
4	S	401	NAG	C3-C2-N2	-2.56	107.79	111.62
4	T	402	NAG	O5-C5-C6	2.51	109.62	106.98
5	R	402	POV	O12-P-O14	-2.47	107.01	112.74
5	T	401	POV	O31-C31-C32	2.47	119.45	111.90
8	T	403	LMT	C2'-C3'-C4'	2.42	114.84	109.59
5	Q	401	POV	C2-O21-C21	-2.39	112.24	117.86
8	T	403	LMT	O5'-C5'-C4'	2.39	114.72	109.71
8	C	402	LMT	C1B-C2B-C3B	2.33	114.49	109.99
8	T	403	LMT	O5B-C5B-C4B	2.24	113.90	109.73
8	C	402	LMT	C1B-O1B-C4'	-2.23	112.33	118.00
8	S	402	LMT	C4B-C3B-C2B	2.22	114.90	110.80
8	B	403	LMT	O3'-C3'-C2'	-2.21	105.42	110.36
8	B	403	LMT	C3B-C4B-C5B	2.18	114.09	110.17
8	B	403	LMT	C1B-C2B-C3B	2.18	114.21	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	402	LMT	C1B-C2B-C3B	2.16	114.17	109.99
8	D	403	LMT	C1B-C2B-C3B	2.13	114.11	109.99
8	E	402	LMT	C1B-O1B-C4'	-2.12	112.62	118.00
5	T	401	POV	C11-C12-N	-2.12	108.50	115.85
4	B	402	NAG	C2-N2-C7	-2.11	120.84	123.39
5	P	403	POV	C11-C12-N	-2.11	108.53	115.85
8	E	402	LMT	C3'-C4'-C5'	2.08	115.50	110.86
4	S	401	NAG	O5-C5-C4	2.04	113.24	110.65
4	E	401	NAG	O5-C5-C6	2.03	109.11	106.98
5	R	402	POV	O13-P-O12	-2.00	108.54	112.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	401	POV	C2-O21-C21-C22
4	T	402	NAG	O7-C7-N2-C2

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	342/347 (98%)	-0.03	1 (0%) 91 58	56, 102, 165, 226	0
1	B	341/347 (98%)	-0.07	0 100 100	58, 109, 175, 270	0
1	C	340/347 (97%)	-0.07	0 100 100	58, 106, 185, 251	0
1	D	340/347 (97%)	-0.10	0 100 100	54, 106, 170, 263	0
1	E	340/347 (97%)	-0.07	0 100 100	57, 105, 170, 230	0
1	P	340/347 (97%)	-0.09	0 100 100	51, 93, 156, 239	0
1	Q	340/347 (97%)	-0.10	0 100 100	58, 99, 167, 242	0
1	R	340/347 (97%)	-0.12	0 100 100	58, 97, 158, 274	0
1	S	340/347 (97%)	-0.07	0 100 100	53, 89, 144, 247	0
1	T	340/347 (97%)	-0.09	0 100 100	49, 88, 151, 210	0
2	F	221/224 (98%)	-0.10	0 100 100	68, 113, 202, 265	0
2	G	222/224 (99%)	0.04	1 (0%) 88 46	75, 142, 230, 309	0
2	H	223/224 (99%)	-0.11	2 (0%) 81 32	52, 100, 158, 275	0
2	I	222/224 (99%)	-0.16	0 100 100	63, 105, 192, 239	0
2	J	222/224 (99%)	0.11	5 (2%) 57 13	64, 146, 281, 313	0
2	U	221/224 (98%)	0.26	5 (2%) 57 13	75, 131, 220, 317	0
2	V	224/224 (100%)	-0.10	2 (0%) 81 32	70, 117, 169, 269	0
2	W	224/224 (100%)	-0.15	1 (0%) 90 51	68, 102, 155, 257	0
2	X	224/224 (100%)	-0.07	2 (0%) 81 32	57, 98, 169, 249	0
2	Y	221/224 (98%)	0.09	2 (0%) 81 32	64, 127, 195, 277	0
3	K	210/215 (97%)	-0.04	1 (0%) 88 46	59, 114, 222, 295	0
3	L	211/215 (98%)	-0.17	0 100 100	49, 91, 170, 224	0
3	M	210/215 (97%)	0.20	9 (4%) 34 7	69, 130, 248, 270	0
3	N	211/215 (98%)	-0.13	0 100 100	66, 116, 158, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	O	211/215 (98%)	-0.14	0 100 100	65, 108, 143, 157	0
3	Z	215/215 (100%)	0.03	1 (0%) 88 46	71, 120, 160, 199	0
3	f	215/215 (100%)	-0.18	1 (0%) 88 46	69, 104, 153, 231	0
3	g	211/215 (98%)	-0.00	0 100 100	71, 127, 173, 218	0
3	h	211/215 (98%)	-0.05	0 100 100	75, 137, 177, 249	0
3	i	214/215 (99%)	-0.13	0 100 100	60, 99, 135, 165	0
All	All	7746/7860 (98%)	-0.06	33 (0%) 90 51	49, 107, 191, 317	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	140	GLN	5.0
2	V	139	ALA	3.3
2	X	142	ASN	3.0
2	J	166	GLY	3.0
3	M	189	GLU	3.0
2	J	165	SER	2.9
2	U	1	GLU	2.8
3	M	183	LEU	2.8
2	J	218	LYS	2.7
3	M	123	PRO	2.7
3	M	122	PRO	2.6
2	U	161	VAL	2.5
3	M	194	TYR	2.5
3	K	123	PRO	2.4
2	H	138	ALA	2.4
2	J	147	LEU	2.4
2	J	168	LEU	2.4
3	M	188	TRP	2.4
3	M	163	GLU	2.4
2	Y	1	GLU	2.3
2	Y	136	GLY	2.3
2	W	139	ALA	2.3
3	M	130	THR	2.3
2	U	192	VAL	2.3
2	G	149	CYS	2.2
3	f	155	GLY	2.2
2	U	191	THR	2.2
3	Z	205	VAL	2.2
2	U	149	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	M	162	MET	2.1
1	A	341	HIS	2.0
2	X	224	CYS	2.0
2	H	1	GLU	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	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	POV	Q	401	46/52	0.74	12.57	108,149,198,237	0
5	POV	D	401	26/52	0.74	6.99	125,176,201,334	0
5	POV	T	401	43/52	0.54	5.81	77,129,177,205	0
8	LMT	E	402	23/35	0.62	4.85	218,239,254,257	0
5	POV	A	402	23/52	0.58	4.60	137,177,208,241	0
5	POV	R	402	35/52	0.40	4.26	96,123,186,208	0
8	LMT	D	403	23/35	0.60	4.12	196,218,239,247	0
5	POV	P	403	42/52	0.37	3.71	82,125,179,206	0
8	LMT	T	403	23/35	0.35	3.68	156,202,217,222	0
5	POV	R	401	34/52	0.36	3.39	99,146,200,535	0
8	LMT	S	402	23/35	0.53	2.81	169,214,224,235	0
4	NAG	S	401	14/15	0.27	2.49	153,184,189,195	0
4	NAG	T	402	14/15	0.34	2.47	153,200,210,211	0
4	NAG	E	401	14/15	0.28	2.17	157,190,206,212	0
4	NAG	C	401	14/15	0.37	1.74	191,210,218,223	0
7	GOL	B	401	6/6	0.37	1.34	115,145,151,167	0
8	LMT	P	402	23/35	0.36	1.01	221,221,221,221	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	B	402	14/15	0.21	0.96	139,168,176,177	0
4	NAG	Q	402	14/15	0.31	0.87	146,184,202,207	0
8	LMT	B	403	23/35	0.46	0.85	176,217,235,242	0
4	NAG	A	401	14/15	0.27	0.33	137,181,192,196	0
8	LMT	C	402	23/35	0.36	0.33	179,179,179,179	0
4	NAG	D	402	14/15	0.20	0.25	153,197,214,221	0
6	CL	P	404	1/1	0.20	-3.10	90,90,90,90	0
6	CL	A	403	1/1	0.78	-	119,119,119,119	0
4	NAG	P	401	14/15	0.28	-	133,182,192,201	0

6.5 Other polymers

There are no such residues in this entry.