wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2014 – 11:44 AM EDT

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 wwPDB validation summary 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

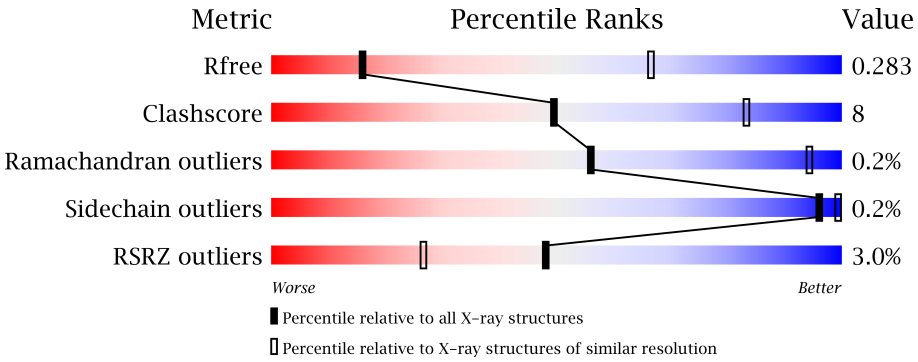
The following versions of software and data (see references) were used in the production of this report:

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 3.60 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}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)

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	P	401	-	X
4	NAG	S	401	-	X
6	FLC	T	403	-	X
7	CL	P	403	-	X
7	CL	P	404	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 60408 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	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

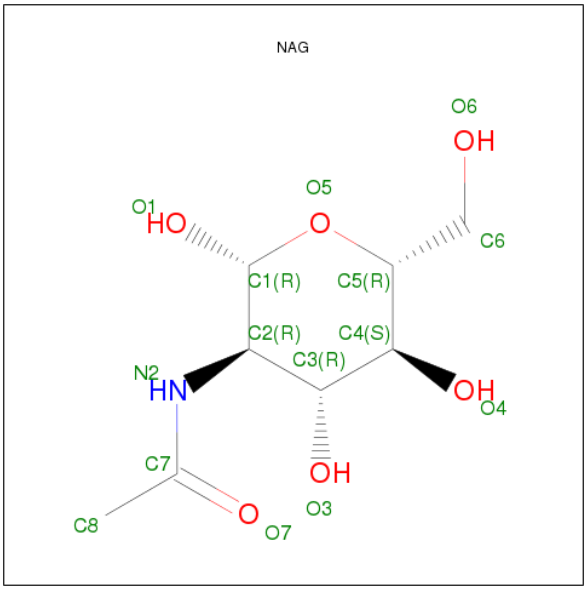
- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

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.

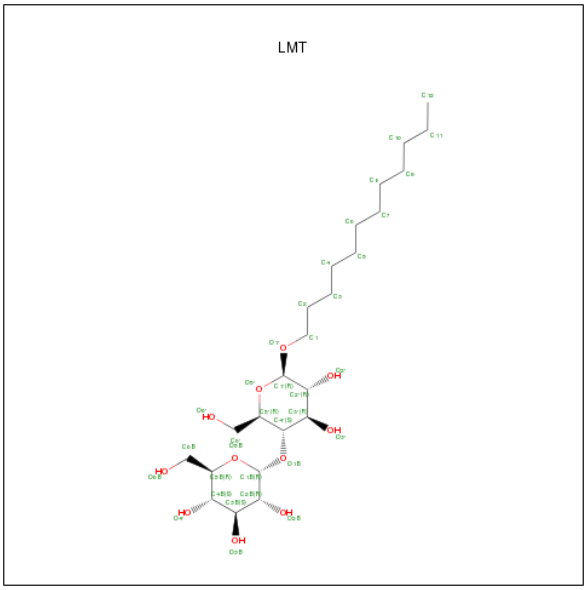
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	212	Total	C	N	O	S	0	0	0
			1606	1008	271	321	6			
3	L	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	N	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	O	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	Z	215	Total	C	N	O	S	0	0	0
			1626	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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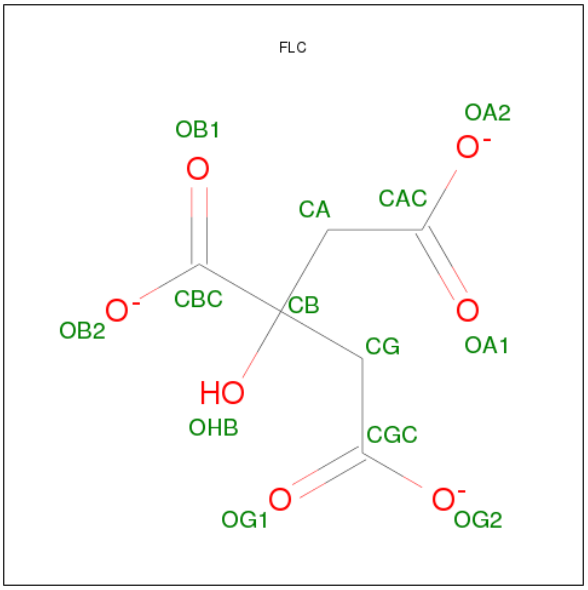
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 23 12 11	0	0
5	C	1	Total C O 23 12 11	0	0
5	D	1	Total C O 23 12 11	0	0
5	E	1	Total C O 23 12 11	0	0
5	P	1	Total C O 23 12 11	0	0
5	Q	1	Total C O 23 12 11	0	0
5	R	1	Total C O 23 12 11	0	0
5	S	1	Total C O 23 12 11	0	0
5	T	1	Total C O 25 14 11	0	0

- 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).

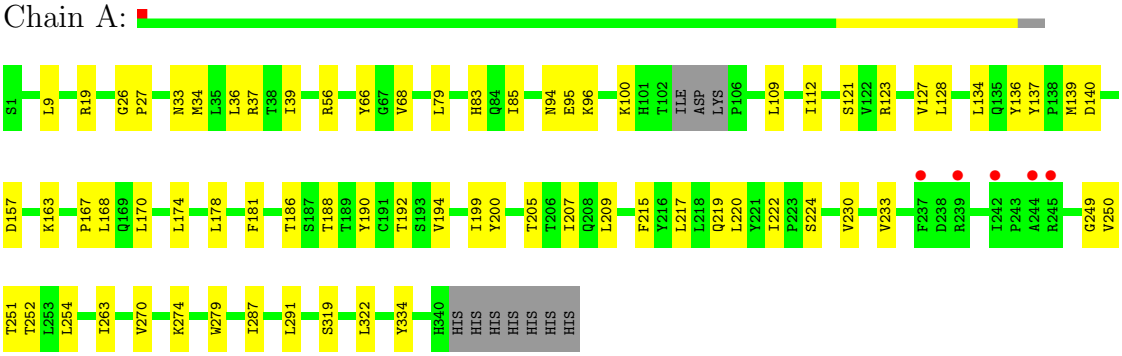
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	P	2	Total Cl 2 2	0	0

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.

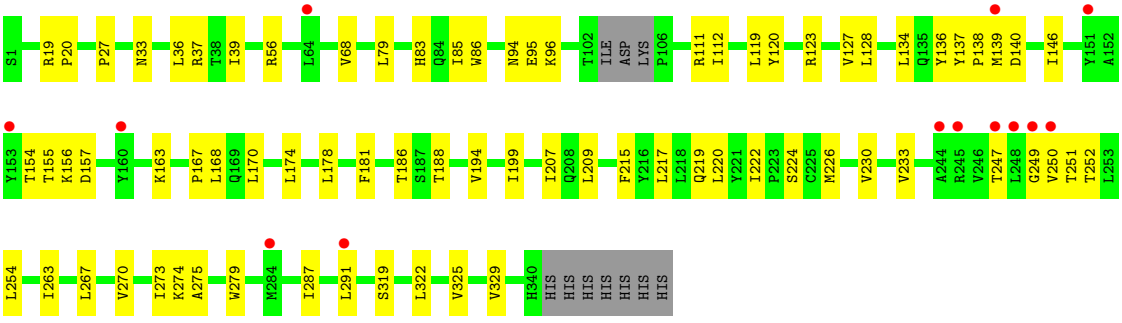
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain A:



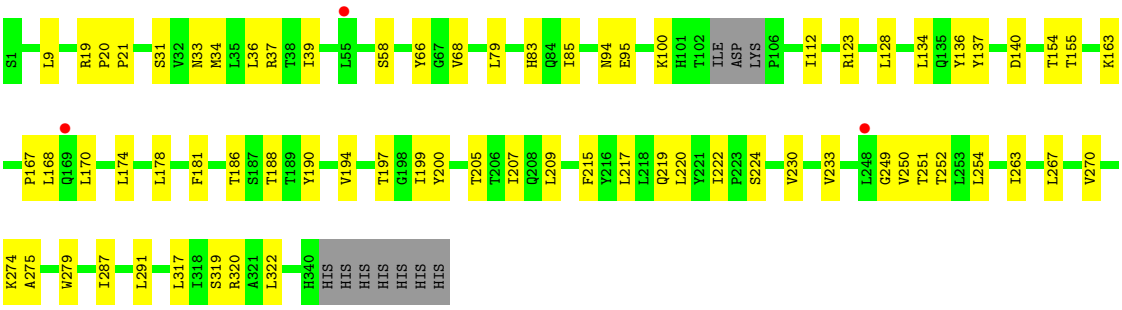
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain B:



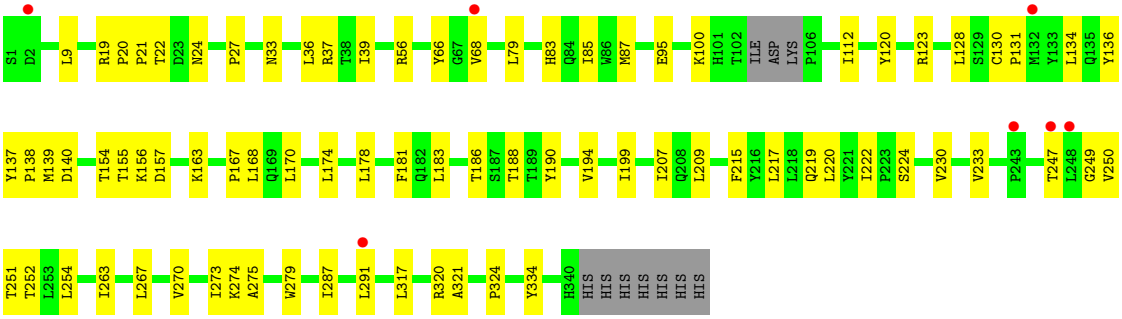
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain C:



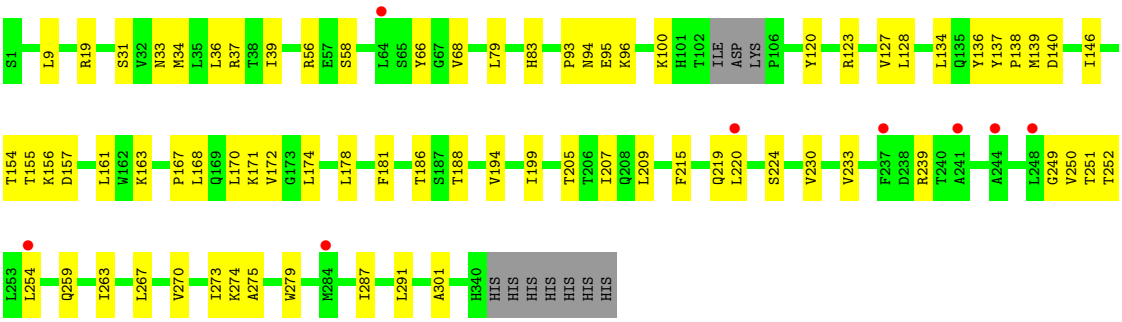
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain D:



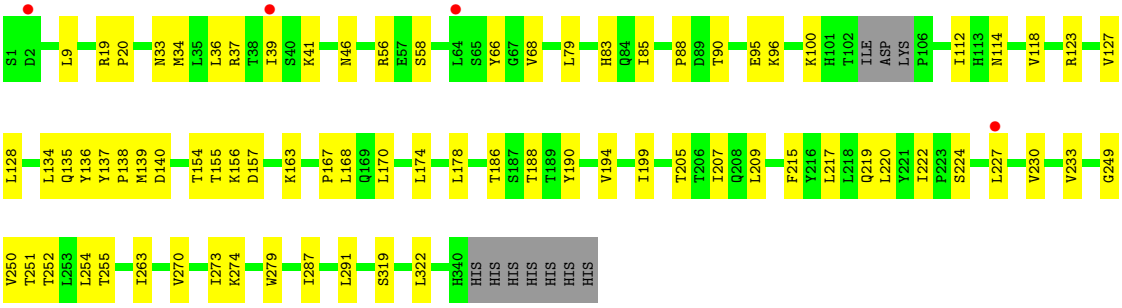
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain E:



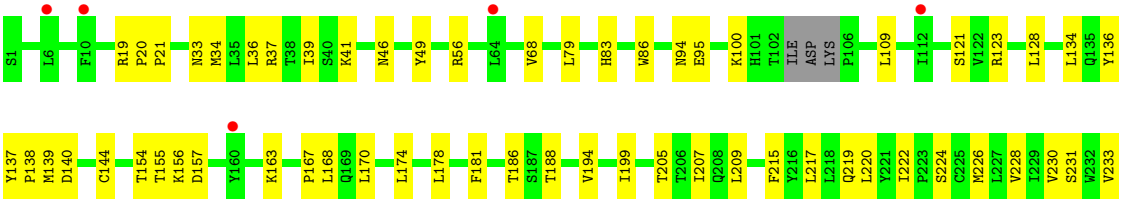
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain P:



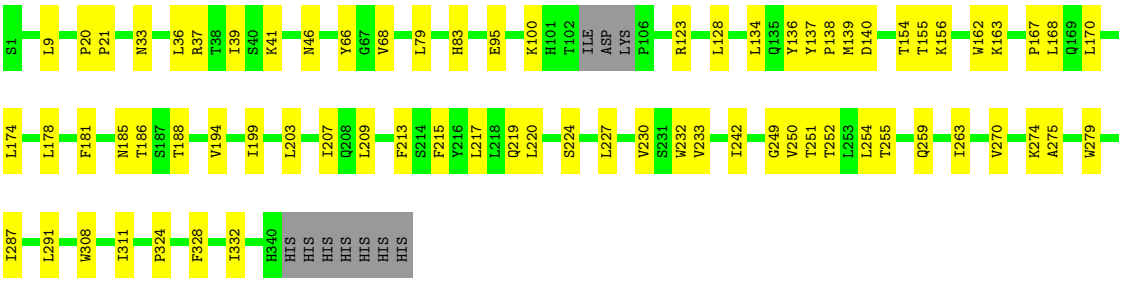
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain Q:



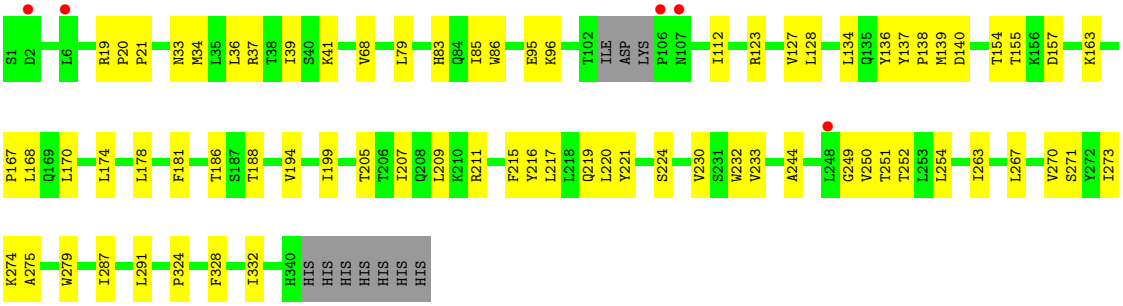
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain R:



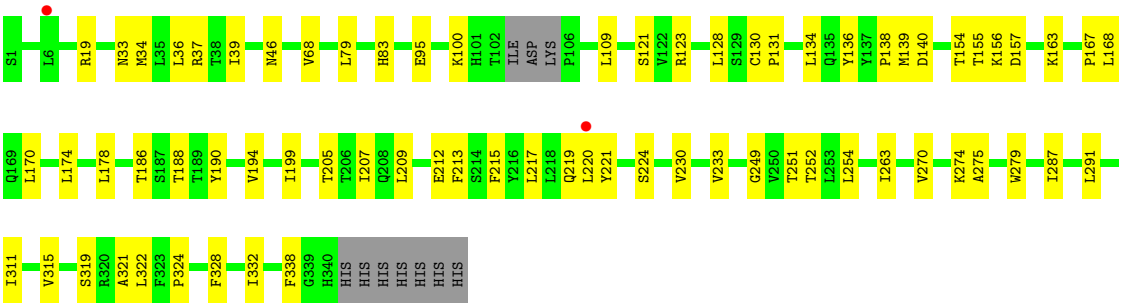
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain S:



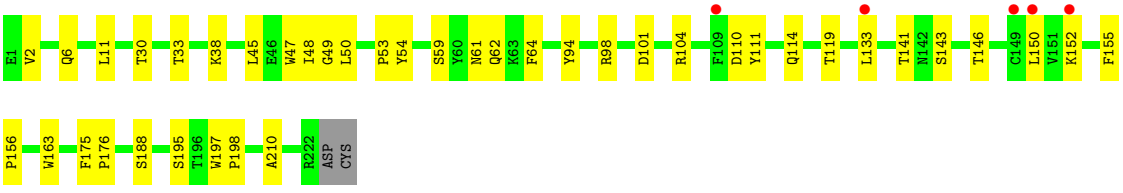
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain T:



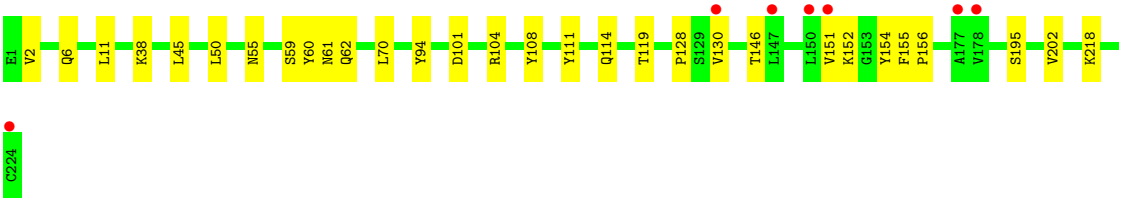
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain F:



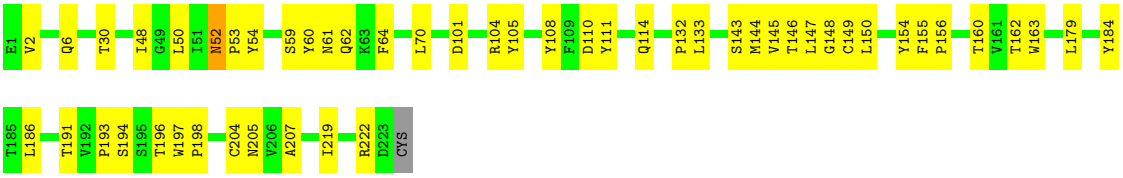
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain G:



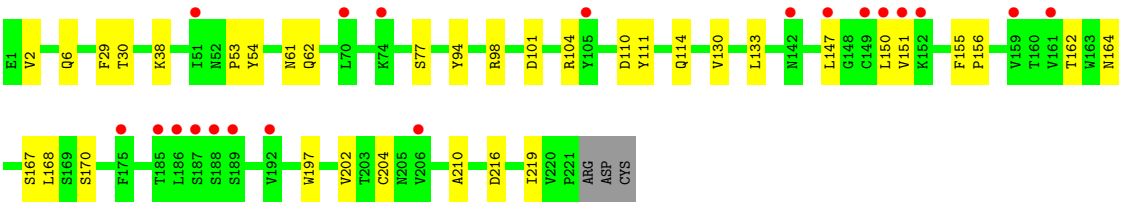
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain H:



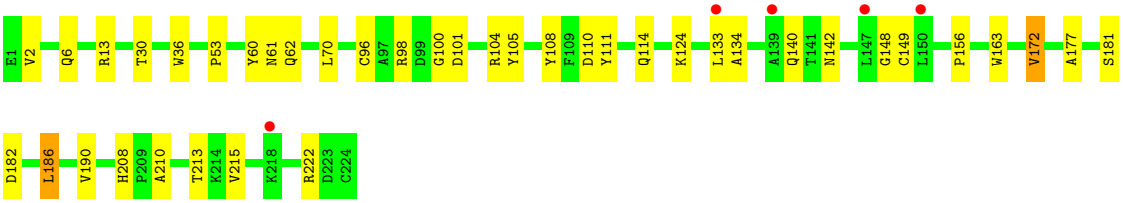
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain U:



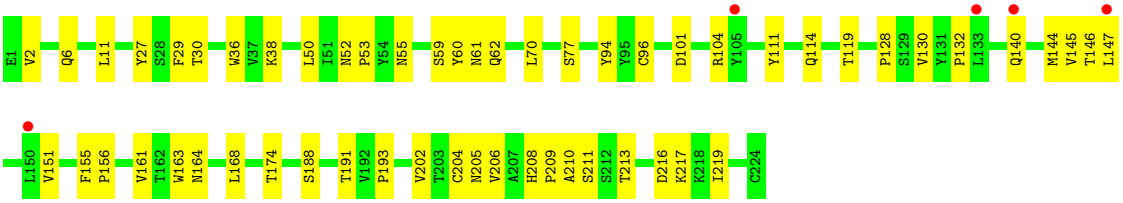
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain V:



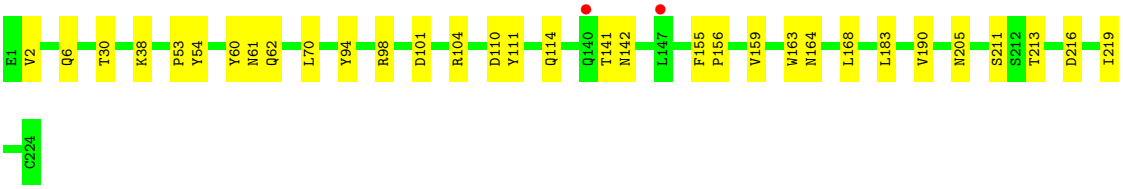
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain W:



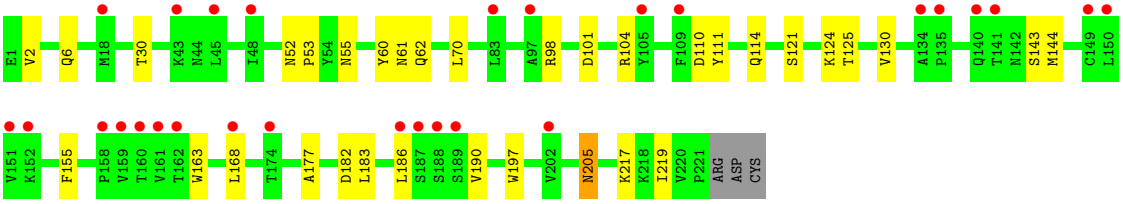
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain X:



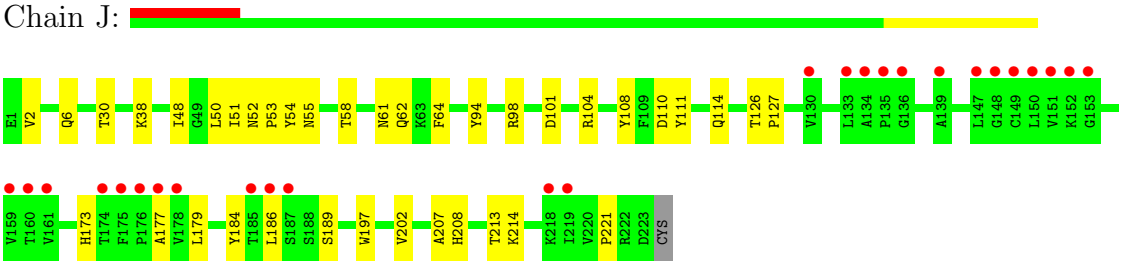
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain Y:



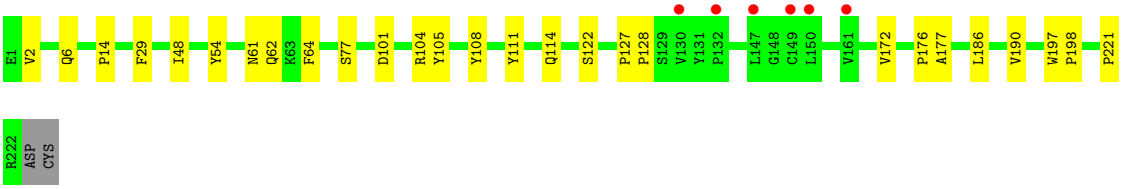
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain J:



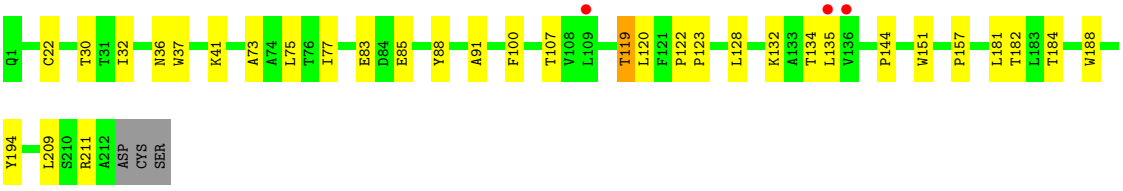
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain I:



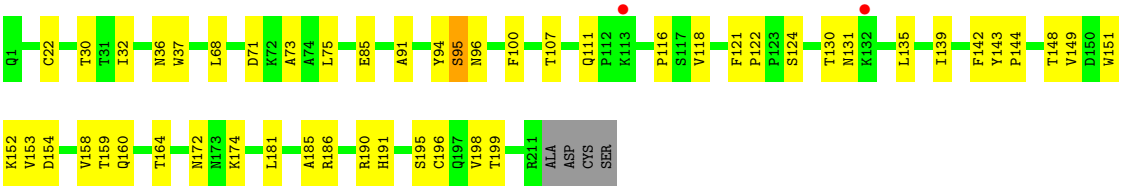
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain K:



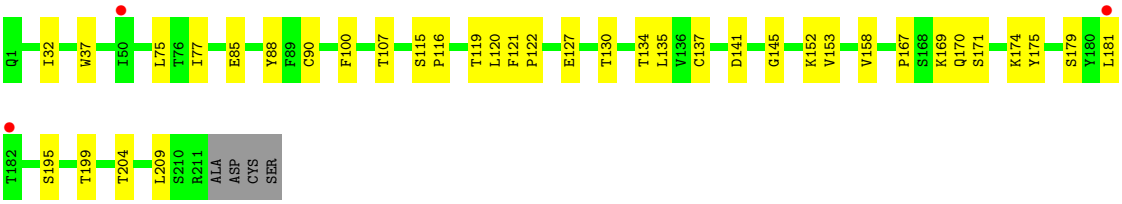
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain L:



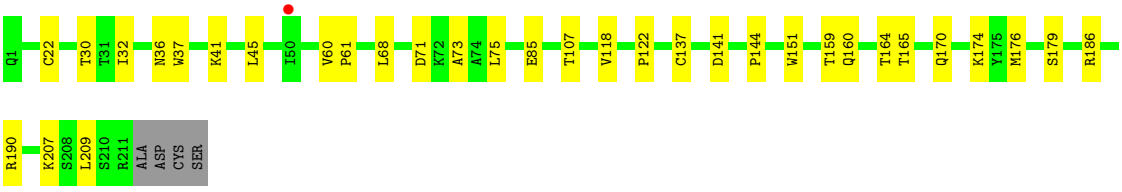
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain N:



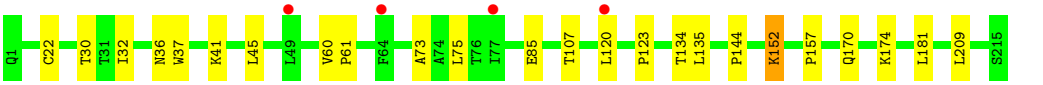
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain O:



• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain Z:

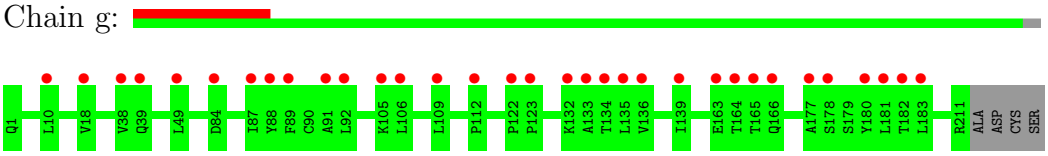


• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain f:

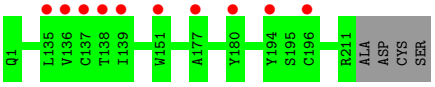
• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain g:



• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain h:

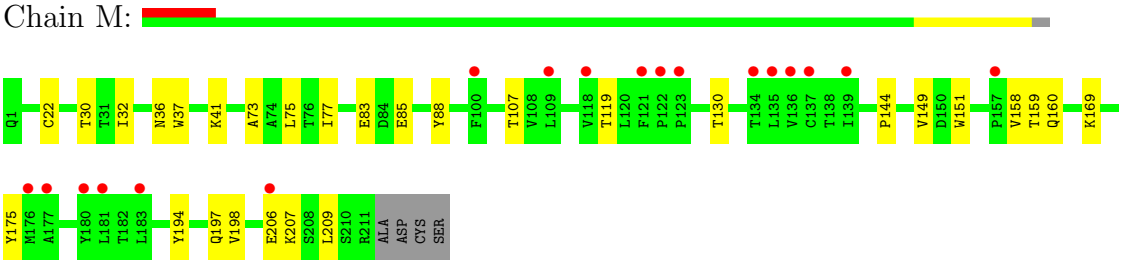


• Molecule 3: Mouse monoclonal Fab fragment, light chain

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	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 0.261 , 0.283	Depositor DCC
R_{free} test set	8778 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	121.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 86.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	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.

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 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	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

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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	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

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 8.

The worst 5 of 827 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	50	92
1	B	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	50	92
1	C	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	50	92
1	D	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	50	92
1	E	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	50	92
1	P	333/347 (96%)	320 (96%)	12 (4%)	1 (0%)	50	92
1	Q	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	50	92
1	R	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	50	92
1	S	333/347 (96%)	320 (96%)	12 (4%)	1 (0%)	50	92
1	T	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	50	92
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%)	38	88
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%)	38	88
3	M	209/215 (97%)	190 (91%)	19 (9%)	0	100	100
3	N	209/215 (97%)	193 (92%)	15 (7%)	1 (0%)	38	88
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%)	38 88
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%)	56 94

5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	192/193 (100%)	190 (99%)	2 (1%)	85 97
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%)	94 98
2	W	193/193 (100%)	193 (100%)	0	100 100
2	X	193/193 (100%)	191 (99%)	2 (1%)	85 97
2	Y	190/193 (98%)	189 (100%)	1 (0%)	94 98
3	K	179/182 (98%)	178 (99%)	1 (1%)	92 98
3	L	179/182 (98%)	177 (99%)	2 (1%)	84 96
3	M	179/182 (98%)	178 (99%)	1 (1%)	92 98
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%)	92 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%)	181 (100%)	0	100 100
All	All	6765/6910 (98%)	6754 (100%)	11 (0%)	96 99

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	130	THR
2	V	186	LEU
2	Y	205	ASN
3	L	71	ASP
2	X	183	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	Z	96	ASN
3	f	96	ASN
3	i	96	ASN

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Mol	Chain	Res	Type
2	Y	205	ASN
3	h	96	ASN

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 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	12,14,15	0.42	0	15,19,21	0.94	1 (6%)
5	LMT	A	402	-	24,24,36	1.37	3 (12%)	34,35,47	1.31	4 (11%)
6	FLC	A	403	-	5,12,12	2.51	2 (40%)	7,17,17	0.69	0
4	NAG	B	401	1	12,14,15	0.86	1 (8%)	15,19,21	0.86	0
5	LMT	B	402	-	24,24,36	1.41	3 (12%)	34,35,47	1.30	5 (14%)
4	NAG	C	401	1	12,14,15	0.44	0	15,19,21	1.79	3 (20%)
5	LMT	C	402	-	24,24,36	1.33	3 (12%)	34,35,47	1.38	6 (17%)
4	NAG	D	401	1	12,14,15	0.67	0	15,19,21	1.04	1 (6%)
5	LMT	D	402	-	24,24,36	1.32	3 (12%)	34,35,47	1.19	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	401	1	12,14,15	0.38	0	15,19,21	0.90	1 (6%)
5	LMT	E	402	-	24,24,36	1.37	3 (12%)	34,35,47	1.17	3 (8%)
4	NAG	P	401	1	12,14,15	0.49	0	15,19,21	1.00	1 (6%)
5	LMT	P	402	-	24,24,36	1.35	3 (12%)	34,35,47	1.19	2 (5%)
4	NAG	Q	401	1	12,14,15	0.79	1 (8%)	15,19,21	0.89	0
5	LMT	Q	402	-	24,24,36	1.34	3 (12%)	34,35,47	1.54	6 (17%)
4	NAG	R	401	1	12,14,15	0.62	0	15,19,21	0.99	1 (6%)
5	LMT	R	402	-	24,24,36	1.33	3 (12%)	34,35,47	1.06	2 (5%)
4	NAG	S	401	1	12,14,15	0.57	0	15,19,21	1.00	1 (6%)
5	LMT	S	402	-	24,24,36	1.34	3 (12%)	34,35,47	1.31	3 (8%)
4	NAG	T	401	1	12,14,15	0.47	0	15,19,21	0.91	1 (6%)
5	LMT	T	402	-	26,26,36	1.26	4 (15%)	36,37,47	1.01	2 (5%)
6	FLC	T	403	-	5,12,12	2.29	2 (40%)	7,17,17	1.32	2 (28%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	T	402	-	-	0/11/51/61	0/2/2/2
6	FLC	T	403	-	-	0/6/16/16	0/0/0/0

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	403	FLC	CA-CAC	4.16	1.52	1.49
6	A	403	FLC	CG-CGC	3.57	1.51	1.49
6	T	403	FLC	CA-CAC	3.53	1.51	1.49
5	Q	402	LMT	O1'-C1'	3.48	1.40	1.23
5	P	402	LMT	O1'-C1'	3.48	1.40	1.23

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	NAG	C2-N2-C7	-4.64	117.78	123.39
5	Q	402	LMT	C2'-C3'-C4'	4.09	118.45	109.59
5	P	402	LMT	C1'-C2'-C3'	3.95	115.64	109.11
5	Q	402	LMT	C1'-C2'-C3'	3.92	115.59	109.11
5	A	402	LMT	O5B-C5B-C4B	3.82	116.83	109.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

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	337/347 (97%)	0.39	5 (1%) 70 43	91, 137, 216, 241	0
1	B	337/347 (97%)	0.40	13 (3%) 37 21	100, 143, 229, 269	0
1	C	337/347 (97%)	0.39	3 (0%) 81 57	94, 140, 228, 260	0
1	D	337/347 (97%)	0.34	7 (2%) 60 35	103, 144, 219, 255	0
1	E	337/347 (97%)	0.41	8 (2%) 56 32	99, 146, 221, 259	0
1	P	337/347 (97%)	0.34	4 (1%) 75 49	92, 110, 180, 204	0
1	Q	337/347 (97%)	0.42	5 (1%) 70 43	88, 110, 175, 199	0
1	R	337/347 (97%)	0.35	0 100 100	87, 105, 166, 183	0
1	S	337/347 (97%)	0.45	5 (1%) 70 43	83, 101, 171, 193	0
1	T	337/347 (97%)	0.35	2 (0%) 86 66	84, 109, 173, 203	0
2	F	222/224 (99%)	0.31	5 (2%) 57 33	112, 139, 215, 248	0
2	G	224/224 (100%)	0.30	7 (3%) 47 26	103, 168, 199, 209	0
2	H	223/224 (99%)	0.24	0 100 100	84, 121, 151, 224	0
2	I	222/224 (99%)	0.21	6 (2%) 52 29	105, 133, 203, 223	0
2	J	223/224 (99%)	0.57	26 (11%) 5 5	115, 163, 263, 278	0
2	U	221/224 (98%)	0.55	20 (9%) 10 7	121, 172, 241, 253	0
2	V	224/224 (100%)	0.26	5 (2%) 59 34	114, 154, 185, 261	0
2	W	224/224 (100%)	0.30	5 (2%) 59 34	102, 126, 145, 207	0
2	X	224/224 (100%)	0.26	2 (0%) 81 57	98, 118, 137, 187	0
2	Y	221/224 (98%)	0.72	28 (12%) 4 4	139, 197, 278, 297	0
3	K	212/215 (98%)	0.25	3 (1%) 72 45	104, 133, 187, 198	0
3	L	211/215 (98%)	0.27	2 (0%) 81 57	81, 109, 162, 172	0
3	M	211/215 (98%)	0.57	18 (8%) 11 7	118, 151, 247, 254	0
3	N	211/215 (98%)	0.16	3 (1%) 72 45	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%)	0.14	1 (0%) 88 71	104, 134, 153, 160	0
3	Z	215/215 (100%)	0.27	4 (1%) 64 37	112, 161, 190, 244	0
3	f	214/215 (99%)	0.23	3 (1%) 72 45	101, 124, 138, 174	0
3	g	211/215 (98%)	0.82	33 (15%) 3 3	150, 223, 274, 281	0
3	h	211/215 (98%)	0.31	10 (4%) 30 17	119, 178, 207, 217	0
3	i	214/215 (99%)	0.22	0 100 100	99, 119, 138, 169	0
All	All	7719/7860 (98%)	0.36	233 (3%) 48 27	81, 134, 233, 297	0

The worst 5 of 233 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	g	135	LEU	7.9
3	g	164	THR	7.7
3	M	123	PRO	7.6
2	J	150	LEU	7.3
3	M	135	LEU	6.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	CL	P	404	1/1	2.59	78.94	115,115,115,115	0
7	CL	P	403	1/1	1.97	61.09	115,115,115,115	0
4	NAG	P	401	14/15	0.51	5.49	232,232,232,232	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	FLC	T	403	13/13	0.37	3.84	187,187,187,187	0
4	NAG	S	401	14/15	0.39	2.95	218,218,218,218	0
6	FLC	A	403	13/13	0.34	1.79	168,168,168,168	0
5	LMT	R	402	23/35	0.38	0.54	149,149,149,149	0
5	LMT	T	402	25/35	0.36	0.26	145,145,145,145	0
5	LMT	B	402	23/35	0.38	0.22	181,181,181,181	0
5	LMT	C	402	23/35	0.34	0.19	173,173,173,173	0
4	NAG	Q	401	14/15	0.26	0.05	176,176,176,176	0
5	LMT	A	402	23/35	0.25	0.00	211,211,211,211	0
5	LMT	D	402	23/35	0.31	-0.14	189,189,189,189	0
5	LMT	P	402	23/35	0.29	-0.31	149,149,149,149	0
4	NAG	D	401	14/15	0.21	-0.34	204,204,204,204	0
5	LMT	E	402	23/35	0.26	-0.68	177,177,177,177	0
4	NAG	C	401	14/15	0.20	-0.79	158,158,158,158	0
4	NAG	B	401	14/15	0.18	-0.85	172,172,172,172	0
4	NAG	T	401	14/15	0.19	-0.90	182,182,182,182	0
4	NAG	E	401	14/15	0.14	-1.39	170,170,170,170	0
5	LMT	S	402	23/35	0.24	-1.55	130,130,130,130	0
4	NAG	A	401	14/15	0.16	-1.56	165,165,165,165	0
5	LMT	Q	402	23/35	0.19	-1.71	143,143,143,143	0
4	NAG	R	401	14/15	0.17	-1.78	191,191,191,191	0

6.5 Other polymers (i)

There are no such residues in this entry.