



wwPDB X-ray Structure Validation Summary Report ⓘ

May 5, 2016 – 08:14 PM EDT

PDB ID : 5FTU
Title : Tetrameric complex of Latrophilin 3, Unc5D and FLRT2
Authors : Jackson, V.A.; Mehmood, S.; Chavent, M.; Roversi, P.; Carrasquero, M.; del Toro, D.; Seyit-Bremer, G.; Ranaivoson, F.M.; Comoletti, D.; Sansom, M.S.P.; Robinson, C.V.; Klein, R.; Seiradake, E.
Deposited on : 2016-01-15
Resolution : 6.01 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

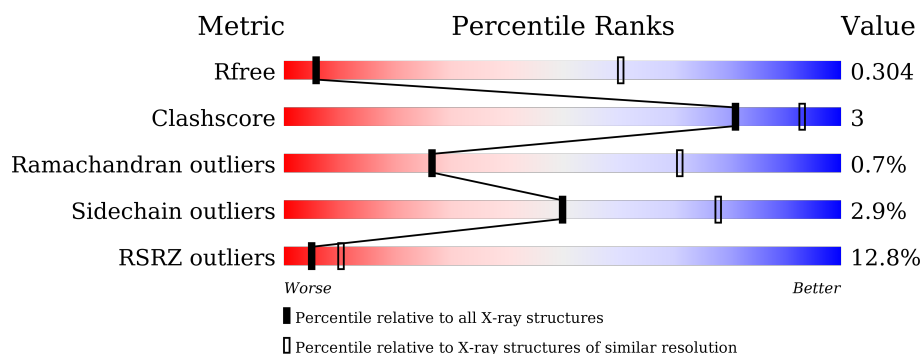
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	139	<div> <div>18%</div> <div>73%</div> <div>24%</div> </div>
1	E	139	<div> <div>15%</div> <div>73%</div> <div>24%</div> </div>
1	I	139	<div> <div>14%</div> <div>73%</div> <div>24%</div> </div>
2	B	339	<div> <div>9%</div> <div>79%</div> <div>17%</div> </div>
2	F	339	<div> <div>7%</div> <div>80%</div> <div>16%</div> </div>
2	J	339	<div> <div>7%</div> <div>78%</div> <div>17%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	383	
3	D	383	
3	G	383	
3	H	383	
3	K	383	
3	L	383	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25680 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NETRIN RECEPTOR UNC5D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			853	536	152	160	5			
1	E	106	Total	C	N	O	S	0	0	0
			853	536	152	160	5			
1	I	106	Total	C	N	O	S	0	0	0
			853	536	152	160	5			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	GLY	-	EXPRESSION TAG	UNP F1LW30
A	163	THR	-	EXPRESSION TAG	UNP F1LW30
A	164	LYS	-	EXPRESSION TAG	UNP F1LW30
A	165	HIS	-	EXPRESSION TAG	UNP F1LW30
A	166	HIS	-	EXPRESSION TAG	UNP F1LW30
A	167	HIS	-	EXPRESSION TAG	UNP F1LW30
A	168	HIS	-	EXPRESSION TAG	UNP F1LW30
A	169	HIS	-	EXPRESSION TAG	UNP F1LW30
A	170	HIS	-	EXPRESSION TAG	UNP F1LW30
E	162	GLY	-	EXPRESSION TAG	UNP F1LW30
E	163	THR	-	EXPRESSION TAG	UNP F1LW30
E	164	LYS	-	EXPRESSION TAG	UNP F1LW30
E	165	HIS	-	EXPRESSION TAG	UNP F1LW30
E	166	HIS	-	EXPRESSION TAG	UNP F1LW30
E	167	HIS	-	EXPRESSION TAG	UNP F1LW30
E	168	HIS	-	EXPRESSION TAG	UNP F1LW30
E	169	HIS	-	EXPRESSION TAG	UNP F1LW30
E	170	HIS	-	EXPRESSION TAG	UNP F1LW30
I	162	GLY	-	EXPRESSION TAG	UNP F1LW30
I	163	THR	-	EXPRESSION TAG	UNP F1LW30
I	164	LYS	-	EXPRESSION TAG	UNP F1LW30
I	165	HIS	-	EXPRESSION TAG	UNP F1LW30
I	166	HIS	-	EXPRESSION TAG	UNP F1LW30

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	167	HIS	-	EXPRESSION TAG	UNP F1LW30
I	168	HIS	-	EXPRESSION TAG	UNP F1LW30
I	169	HIS	-	EXPRESSION TAG	UNP F1LW30
I	170	HIS	-	EXPRESSION TAG	UNP F1LW30

- Molecule 2 is a protein called LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	326	Total	C	N	O	S	0	0	0
			2587	1634	461	478	14			
2	F	326	Total	C	N	O	S	0	0	0
			2587	1634	461	478	14			
2	J	326	Total	C	N	O	S	0	0	0
			2587	1634	461	478	14			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	33	THR	-	EXPRESSION TAG	UNP Q8BLU0
B	34	GLY	-	EXPRESSION TAG	UNP Q8BLU0
B	363	ARG	-	EXPRESSION TAG	UNP Q8BLU0
B	364	THR	-	EXPRESSION TAG	UNP Q8BLU0
B	365	LYS	-	EXPRESSION TAG	UNP Q8BLU0
B	366	HIS	-	EXPRESSION TAG	UNP Q8BLU0
B	367	HIS	-	EXPRESSION TAG	UNP Q8BLU0
B	368	HIS	-	EXPRESSION TAG	UNP Q8BLU0
B	369	HIS	-	EXPRESSION TAG	UNP Q8BLU0
B	370	HIS	-	EXPRESSION TAG	UNP Q8BLU0
B	371	HIS	-	EXPRESSION TAG	UNP Q8BLU0
F	33	THR	-	EXPRESSION TAG	UNP Q8BLU0
F	34	GLY	-	EXPRESSION TAG	UNP Q8BLU0
F	363	ARG	-	EXPRESSION TAG	UNP Q8BLU0
F	364	THR	-	EXPRESSION TAG	UNP Q8BLU0
F	365	LYS	-	EXPRESSION TAG	UNP Q8BLU0
F	366	HIS	-	EXPRESSION TAG	UNP Q8BLU0
F	367	HIS	-	EXPRESSION TAG	UNP Q8BLU0
F	368	HIS	-	EXPRESSION TAG	UNP Q8BLU0
F	369	HIS	-	EXPRESSION TAG	UNP Q8BLU0
F	370	HIS	-	EXPRESSION TAG	UNP Q8BLU0
F	371	HIS	-	EXPRESSION TAG	UNP Q8BLU0
J	33	THR	-	EXPRESSION TAG	UNP Q8BLU0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	34	GLY	-	EXPRESSION TAG	UNP Q8BLU0
J	363	ARG	-	EXPRESSION TAG	UNP Q8BLU0
J	364	THR	-	EXPRESSION TAG	UNP Q8BLU0
J	365	LYS	-	EXPRESSION TAG	UNP Q8BLU0
J	366	HIS	-	EXPRESSION TAG	UNP Q8BLU0
J	367	HIS	-	EXPRESSION TAG	UNP Q8BLU0
J	368	HIS	-	EXPRESSION TAG	UNP Q8BLU0
J	369	HIS	-	EXPRESSION TAG	UNP Q8BLU0
J	370	HIS	-	EXPRESSION TAG	UNP Q8BLU0
J	371	HIS	-	EXPRESSION TAG	UNP Q8BLU0

- Molecule 3 is a protein called ADHESION G PROTEIN-COUPLED RECEPTOR L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2943	1867	485	575	16			
3	D	263	Total	C	N	O	S	0	0	0
			2131	1360	351	415	5			
3	G	365	Total	C	N	O	S	0	0	0
			2943	1867	485	575	16			
3	H	263	Total	C	N	O	S	0	0	0
			2131	1360	351	415	5			
3	K	365	Total	C	N	O	S	0	0	0
			2943	1867	485	575	16			
3	L	263	Total	C	N	O	S	0	0	0
			2131	1360	351	415	5			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	90	THR	-	EXPRESSION TAG	UNP Q80TS3
C	91	GLY	-	EXPRESSION TAG	UNP Q80TS3
C	464	GLY	-	EXPRESSION TAG	UNP Q80TS3
C	465	THR	-	EXPRESSION TAG	UNP Q80TS3
C	466	LYS	-	EXPRESSION TAG	UNP Q80TS3
C	467	HIS	-	EXPRESSION TAG	UNP Q80TS3
C	468	HIS	-	EXPRESSION TAG	UNP Q80TS3
C	469	HIS	-	EXPRESSION TAG	UNP Q80TS3
C	470	HIS	-	EXPRESSION TAG	UNP Q80TS3
C	471	HIS	-	EXPRESSION TAG	UNP Q80TS3
C	472	HIS	-	EXPRESSION TAG	UNP Q80TS3
D	90	THR	-	EXPRESSION TAG	UNP Q80TS3

Continued on next page...

Continued from previous page...

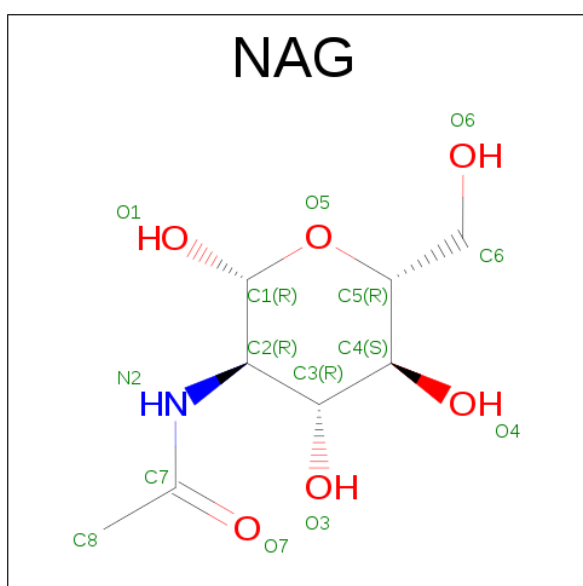
Chain	Residue	Modelled	Actual	Comment	Reference
D	91	GLY	-	EXPRESSION TAG	UNP Q80TS3
D	464	GLY	-	EXPRESSION TAG	UNP Q80TS3
D	465	THR	-	EXPRESSION TAG	UNP Q80TS3
D	466	LYS	-	EXPRESSION TAG	UNP Q80TS3
D	467	HIS	-	EXPRESSION TAG	UNP Q80TS3
D	468	HIS	-	EXPRESSION TAG	UNP Q80TS3
D	469	HIS	-	EXPRESSION TAG	UNP Q80TS3
D	470	HIS	-	EXPRESSION TAG	UNP Q80TS3
D	471	HIS	-	EXPRESSION TAG	UNP Q80TS3
D	472	HIS	-	EXPRESSION TAG	UNP Q80TS3
G	90	THR	-	EXPRESSION TAG	UNP Q80TS3
G	91	GLY	-	EXPRESSION TAG	UNP Q80TS3
G	464	GLY	-	EXPRESSION TAG	UNP Q80TS3
G	465	THR	-	EXPRESSION TAG	UNP Q80TS3
G	466	LYS	-	EXPRESSION TAG	UNP Q80TS3
G	467	HIS	-	EXPRESSION TAG	UNP Q80TS3
G	468	HIS	-	EXPRESSION TAG	UNP Q80TS3
G	469	HIS	-	EXPRESSION TAG	UNP Q80TS3
G	470	HIS	-	EXPRESSION TAG	UNP Q80TS3
G	471	HIS	-	EXPRESSION TAG	UNP Q80TS3
G	472	HIS	-	EXPRESSION TAG	UNP Q80TS3
H	90	THR	-	EXPRESSION TAG	UNP Q80TS3
H	91	GLY	-	EXPRESSION TAG	UNP Q80TS3
H	464	GLY	-	EXPRESSION TAG	UNP Q80TS3
H	465	THR	-	EXPRESSION TAG	UNP Q80TS3
H	466	LYS	-	EXPRESSION TAG	UNP Q80TS3
H	467	HIS	-	EXPRESSION TAG	UNP Q80TS3
H	468	HIS	-	EXPRESSION TAG	UNP Q80TS3
H	469	HIS	-	EXPRESSION TAG	UNP Q80TS3
H	470	HIS	-	EXPRESSION TAG	UNP Q80TS3
H	471	HIS	-	EXPRESSION TAG	UNP Q80TS3
H	472	HIS	-	EXPRESSION TAG	UNP Q80TS3
K	90	THR	-	EXPRESSION TAG	UNP Q80TS3
K	91	GLY	-	EXPRESSION TAG	UNP Q80TS3
K	464	GLY	-	EXPRESSION TAG	UNP Q80TS3
K	465	THR	-	EXPRESSION TAG	UNP Q80TS3
K	466	LYS	-	EXPRESSION TAG	UNP Q80TS3
K	467	HIS	-	EXPRESSION TAG	UNP Q80TS3
K	468	HIS	-	EXPRESSION TAG	UNP Q80TS3
K	469	HIS	-	EXPRESSION TAG	UNP Q80TS3
K	470	HIS	-	EXPRESSION TAG	UNP Q80TS3
K	471	HIS	-	EXPRESSION TAG	UNP Q80TS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	472	HIS	-	EXPRESSION TAG	UNP Q80TS3
L	90	THR	-	EXPRESSION TAG	UNP Q80TS3
L	91	GLY	-	EXPRESSION TAG	UNP Q80TS3
L	464	GLY	-	EXPRESSION TAG	UNP Q80TS3
L	465	THR	-	EXPRESSION TAG	UNP Q80TS3
L	466	LYS	-	EXPRESSION TAG	UNP Q80TS3
L	467	HIS	-	EXPRESSION TAG	UNP Q80TS3
L	468	HIS	-	EXPRESSION TAG	UNP Q80TS3
L	469	HIS	-	EXPRESSION TAG	UNP Q80TS3
L	470	HIS	-	EXPRESSION TAG	UNP Q80TS3
L	471	HIS	-	EXPRESSION TAG	UNP Q80TS3
L	472	HIS	-	EXPRESSION TAG	UNP Q80TS3

- 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	14	0
			14	8	1	5		
4	C	1	Total	C	N	O	14	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	14	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	14	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	14	0
			14	8	1	5		
4	K	1	Total	C	N	O	14	0
			14	8	1	5		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		
5	K	1	Total	Na	0	0
			1	1		
5	H	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		
5	L	1	Total	Na	0	0
			1	1		

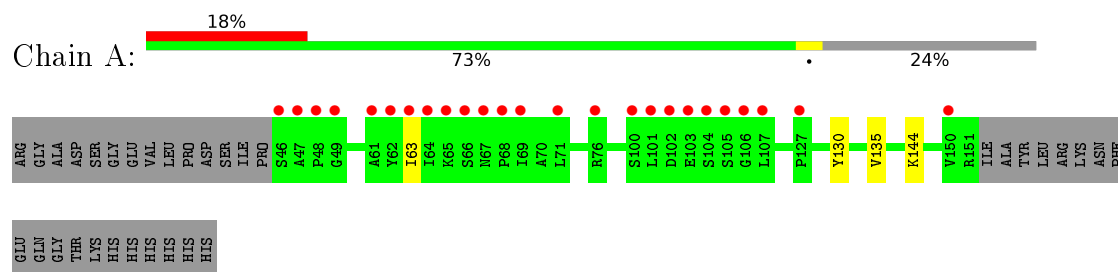
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	K	1	Total	Ca	0	0
			1	1		
6	H	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	L	1	Total	Ca	0	0
			1	1		

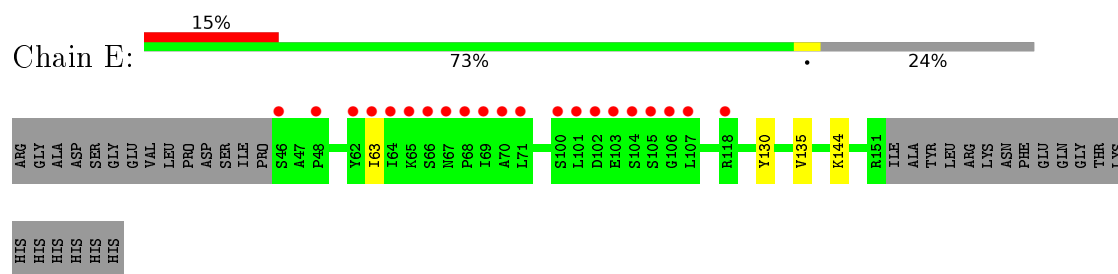
3 Residue-property plots [i](#)

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.

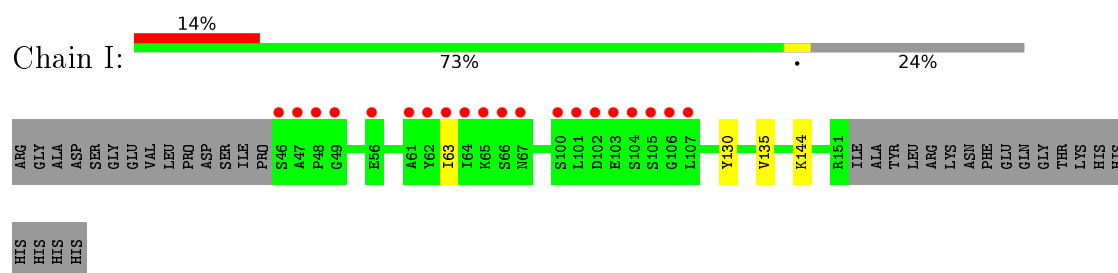
• Molecule 1: NETRIN RECEPTOR UNC5D



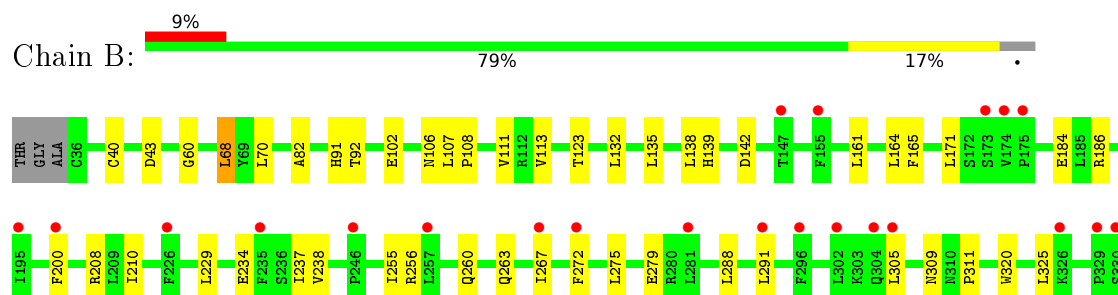
• Molecule 1: NETRIN RECEPTOR UNC5D

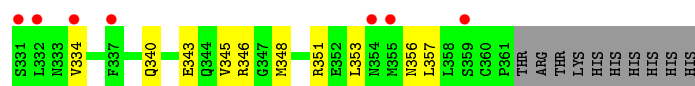


• Molecule 1: NETRIN RECEPTOR UNC5D

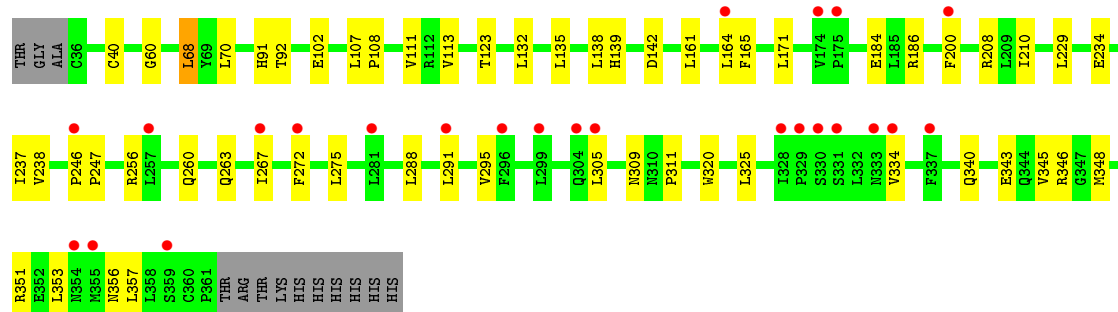
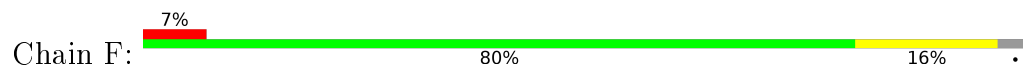


• Molecule 2: LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2

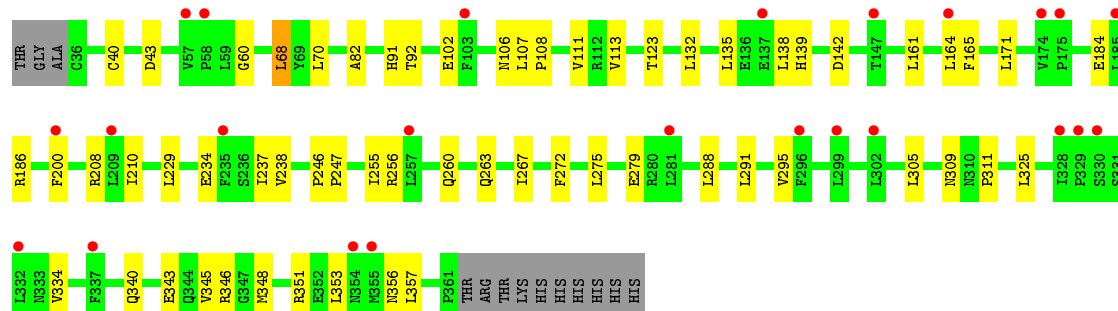
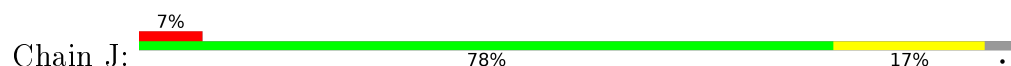




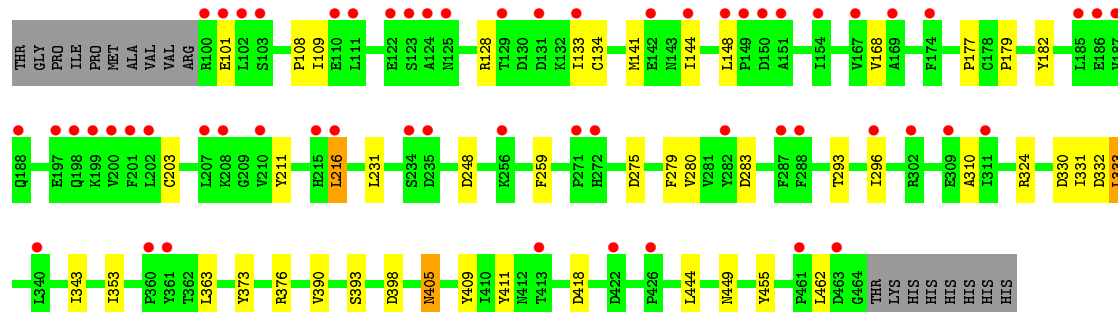
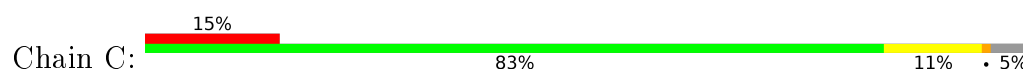
• Molecule 2: LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2



• Molecule 2: LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2

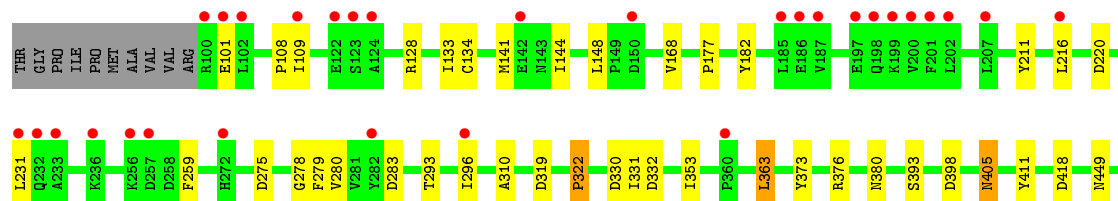


• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3



• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3





L462
D463
G464
THR
LYS
HIS
HIS
HIS
HIS
HIS

● Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3



THR	GLY	PRO	ILE	PRO	MET	ALA	VAL	VAL	ARG	ARG	ASN	GLU	LEU	SER	CYS	GLU	SER	TYR	PRO	PRO	ILE	GLU	LEU	ARG	CYS	PRO	GLY	THR	ASP	VAL	ILE	MET	ILE	GLU	SER	ALA	ASN	TYR	GLY	ARG	THR	ASP	GLN	ARG	CYS	TYR	LEU	PRO	
ASP	ALA	TYR	LYS	ILE	MET	SER	GLN	ARG	CYS	ASN	ASN	ARG	THR	GLN	CYS	ALA	VAL	VAL	VAL	ALA	GLY	PRO	ASP	VAL	PHE	PRO	ASP	PRO	CYS	PRO	GLY	THR	TYR	LYS	TYR	LEU	GLU	VAL	GLN	THR	LYS	VAL	PHE	L202	L207	A225	W226	C227	K228
L231	Y238	L250	Y268	K269	L270	P271	H272	D275	F279	V280	V281	Y282	D283	G284	A285	L286	F287	F288	R292	T293	I296	V297	K298	F299	D300	L301	R302	T303	R304	I305	K306	S307	G308	E309	A310	I311	I312	A313	P322	L333	A334	V335	V342	I343	I353	L358			
K359	F360	T361	T362	L363	R364	Y373	N380	A381	F382	K383	T389	V390	K406	Y409	I410	Y411	D418	P424	F425	S428	V435	D436	I444	L457	G464	THR	LYS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS			

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	292.36 Å 292.36 Å 291.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	206.73 – 6.01 146.18 – 6.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (206.73-6.01) 97.3 (146.18-6.00)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 6.20 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.276 , 0.278 0.282 , 0.304	Depositor DCC
R_{free} test set	719 reflections (4.56%)	DCC
Wilson B-factor (Å ²)	344.8	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 316.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.360 for l,-k,h 0.356 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	25680	wwPDB-VP
Average B, all atoms (Å ²)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/876	0.49	0/1186
1	E	0.35	0/876	0.49	0/1186
1	I	0.35	0/876	0.49	0/1186
2	B	0.38	0/2637	0.57	0/3583
2	F	0.38	0/2637	0.56	0/3583
2	J	0.38	0/2637	0.56	0/3583
3	C	0.37	0/3021	0.56	0/4115
3	D	0.35	0/2189	0.51	0/2982
3	G	0.36	0/3021	0.54	0/4115
3	H	0.35	0/2189	0.51	0/2982
3	K	0.36	0/3021	0.54	0/4115
3	L	0.35	0/2189	0.52	0/2982
All	All	0.36	0/26169	0.54	0/35598

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	853	0	814	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	853	0	814	1	0
1	I	853	0	814	1	0
2	B	2587	0	2602	28	0
2	F	2587	0	2602	26	0
2	J	2587	0	2602	28	0
3	C	2943	0	2797	18	0
3	D	2131	0	2017	14	0
3	G	2943	0	2797	13	0
3	H	2131	0	2017	15	0
3	K	2943	0	2797	16	0
3	L	2131	0	2017	13	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
4	G	14	0	13	0	0
4	I	14	0	13	0	0
4	J	14	0	13	0	0
4	K	14	0	13	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
All	All	25680	0	24807	167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 167 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:393:SER:HA	3:G:405:ASN:H	1.55	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:393:SER:HA	3:C:405:ASN:H	1.56	0.69
3:K:393:SER:HA	3:K:405:ASN:H	1.61	0.65
3:C:128:ARG:HH22	3:C:134:CYS:HB2	1.65	0.62
3:K:128:ARG:HH22	3:K:134:CYS:HB2	1.65	0.61

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	104/139 (75%)	101 (97%)	2 (2%)	1 (1%)	19	65
1	E	104/139 (75%)	101 (97%)	2 (2%)	1 (1%)	19	65
1	I	104/139 (75%)	101 (97%)	2 (2%)	1 (1%)	19	65
2	B	322/339 (95%)	285 (88%)	35 (11%)	2 (1%)	30	74
2	F	322/339 (95%)	285 (88%)	35 (11%)	2 (1%)	30	74
2	J	322/339 (95%)	285 (88%)	35 (11%)	2 (1%)	30	74
3	C	363/383 (95%)	330 (91%)	29 (8%)	4 (1%)	17	63
3	D	259/383 (68%)	241 (93%)	17 (7%)	1 (0%)	39	80
3	G	363/383 (95%)	334 (92%)	27 (7%)	2 (1%)	30	74
3	H	259/383 (68%)	241 (93%)	17 (7%)	1 (0%)	39	80
3	K	363/383 (95%)	334 (92%)	26 (7%)	3 (1%)	24	69
3	L	259/383 (68%)	241 (93%)	17 (7%)	1 (0%)	39	80
All	All	3144/3732 (84%)	2879 (92%)	244 (8%)	21 (1%)	26	71

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	248	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	216	LEU
2	B	309	ASN
3	C	449	ASN
2	F	309	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	94/122 (77%)	93 (99%)	1 (1%)	80	91
1	E	94/122 (77%)	93 (99%)	1 (1%)	80	91
1	I	94/122 (77%)	93 (99%)	1 (1%)	80	91
2	B	297/308 (96%)	288 (97%)	9 (3%)	48	77
2	F	297/308 (96%)	288 (97%)	9 (3%)	48	77
2	J	297/308 (96%)	288 (97%)	9 (3%)	48	77
3	C	324/340 (95%)	310 (96%)	14 (4%)	35	70
3	D	231/340 (68%)	227 (98%)	4 (2%)	68	87
3	G	324/340 (95%)	312 (96%)	12 (4%)	41	73
3	H	231/340 (68%)	227 (98%)	4 (2%)	68	87
3	K	324/340 (95%)	311 (96%)	13 (4%)	38	71
3	L	231/340 (68%)	226 (98%)	5 (2%)	60	83
All	All	2838/3330 (85%)	2756 (97%)	82 (3%)	50	78

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	357	LEU
3	G	330	ASP
3	K	405	ASN
3	G	141	MET
3	G	275	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	293	GLN
2	F	354	ASN
2	J	293	GLN
2	F	72	ASN
2	J	310	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 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	1152	-	14,14,15	0.41	0	15,19,21	1.20	1 (6%)
4	NAG	B	1362	-	14,14,15	0.43	0	15,19,21	1.17	1 (6%)
4	NAG	C	1465	-	14,14,15	0.51	0	15,19,21	0.96	1 (6%)
4	NAG	E	1152	-	14,14,15	0.42	0	15,19,21	1.19	1 (6%)
4	NAG	F	1362	-	14,14,15	0.43	0	15,19,21	1.16	1 (6%)
4	NAG	G	1465	-	14,14,15	0.52	0	15,19,21	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	I	1152	-	14,14,15	0.40	0	15,19,21	1.20	1 (6%)
4	NAG	J	1362	-	14,14,15	0.43	0	15,19,21	1.16	1 (6%)
4	NAG	K	1465	-	14,14,15	0.51	0	15,19,21	0.94	1 (6%)

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	1152	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1362	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1465	-	-	0/6/23/26	0/1/1/1
4	NAG	E	1152	-	-	0/6/23/26	0/1/1/1
4	NAG	F	1362	-	-	0/6/23/26	0/1/1/1
4	NAG	G	1465	-	-	0/6/23/26	0/1/1/1
4	NAG	I	1152	-	-	0/6/23/26	0/1/1/1
4	NAG	J	1362	-	-	0/6/23/26	0/1/1/1
4	NAG	K	1465	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1152	NAG	C4-C3-C2	-2.51	107.44	111.34
4	E	1152	NAG	C4-C3-C2	-2.50	107.46	111.34
4	A	1152	NAG	C4-C3-C2	-2.49	107.48	111.34
4	J	1362	NAG	C4-C3-C2	-2.43	107.56	111.34
4	B	1362	NAG	C4-C3-C2	-2.42	107.58	111.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	106/139 (76%)	1.10	25 (23%) 1 5	162, 191, 238, 249	0
1	E	106/139 (76%)	0.88	21 (19%) 1 6	162, 191, 238, 249	0
1	I	106/139 (76%)	0.84	20 (18%) 2 7	162, 191, 238, 249	0
2	B	326/339 (96%)	0.15	29 (8%) 12 16	127, 162, 226, 250	0
2	F	326/339 (96%)	0.05	24 (7%) 17 20	127, 162, 226, 250	0
2	J	326/339 (96%)	0.07	24 (7%) 17 20	127, 162, 226, 250	0
3	C	365/383 (95%)	0.73	58 (15%) 3 8	112, 152, 257, 274	0
3	D	263/383 (68%)	0.19	25 (9%) 10 14	187, 227, 271, 278	0
3	G	365/383 (95%)	0.48	44 (12%) 6 11	112, 152, 257, 274	0
3	H	263/383 (68%)	0.71	50 (19%) 2 7	187, 227, 271, 278	0
3	K	365/383 (95%)	0.31	30 (8%) 14 18	112, 152, 257, 274	0
3	L	263/383 (68%)	0.89	56 (21%) 1 6	187, 227, 271, 278	0
All	All	3180/3732 (85%)	0.44	406 (12%) 5 10	112, 181, 264, 278	0

The worst 5 of 406 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	102	ASP	10.4
1	I	48	PRO	9.6
1	E	102	ASP	9.4
3	H	309	GLU	9.0
1	A	48	PRO	8.9

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	CA	K	1467	1/1	0.80	0.24	-0.48	138,138,138,138	0
5	NA	D	1465	1/1	0.94	0.28	-0.67	221,221,221,221	0
6	CA	G	1467	1/1	0.82	0.20	-0.69	138,138,138,138	0
5	NA	G	1466	1/1	0.90	0.18	-0.86	136,136,136,136	0
6	CA	H	1466	1/1	0.48	0.25	-0.89	221,221,221,221	0
6	CA	D	1466	1/1	0.43	0.18	-1.07	221,221,221,221	0
6	CA	C	1467	1/1	0.89	0.14	-1.30	138,138,138,138	0
5	NA	K	1466	1/1	0.78	0.16	-1.40	136,136,136,136	0
5	NA	H	1465	1/1	0.83	0.20	-1.45	221,221,221,221	0
6	CA	L	1466	1/1	0.67	0.16	-1.48	221,221,221,221	0
5	NA	L	1465	1/1	0.97	0.21	-1.52	221,221,221,221	0
5	NA	C	1466	1/1	0.92	0.13	-1.78	136,136,136,136	0
4	NAG	C	1465	14/15	-	-	-	256,264,272,272	14
4	NAG	K	1465	14/15	-	-	-	256,264,272,272	14
4	NAG	A	1152	14/15	0.62	1.32	-	227,230,233,234	0
4	NAG	E	1152	14/15	0.70	1.30	-	227,230,233,234	0
4	NAG	F	1362	14/15	-	-	-	188,192,199,203	14
4	NAG	J	1362	14/15	-	-	-	188,192,199,203	14
4	NAG	B	1362	14/15	-	-	-	188,192,199,203	14
4	NAG	I	1152	14/15	0.71	0.99	-	227,230,233,234	0
4	NAG	G	1465	14/15	-	-	-	256,264,272,272	14

6.5 Other polymers ⓘ

There are no such residues in this entry.