



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

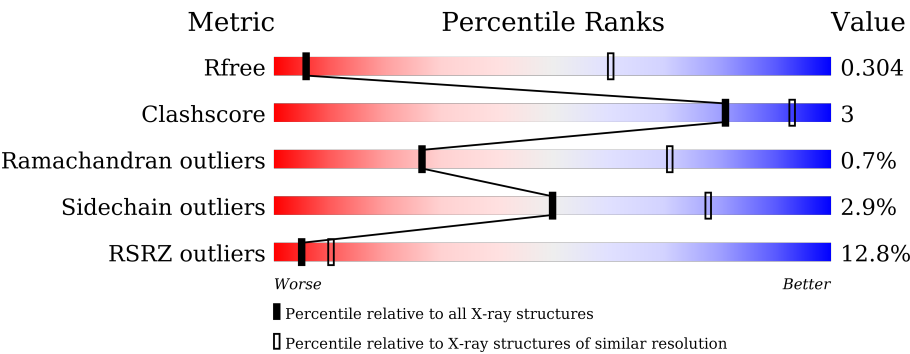
# 1 Overall quality at a glance i

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  $\geq 3$ , 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><div></div><div>73%</div><div></div><div>24%</div></div><div></div></div>
1	E	139	<div><div>15%</div><div><div></div><div>73%</div><div></div><div>24%</div></div><div></div></div>
1	I	139	<div><div>14%</div><div><div></div><div>73%</div><div></div><div>24%</div></div><div></div></div>
2	B	339	<div><div>9%</div><div><div></div><div>79%</div><div></div><div>17%</div></div><div></div></div>
2	F	339	<div><div>7%</div><div><div></div><div>80%</div><div></div><div>16%</div></div><div></div></div>
2	J	339	<div><div>7%</div><div><div></div><div>78%</div><div></div><div>17%</div></div><div></div></div>

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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

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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

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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

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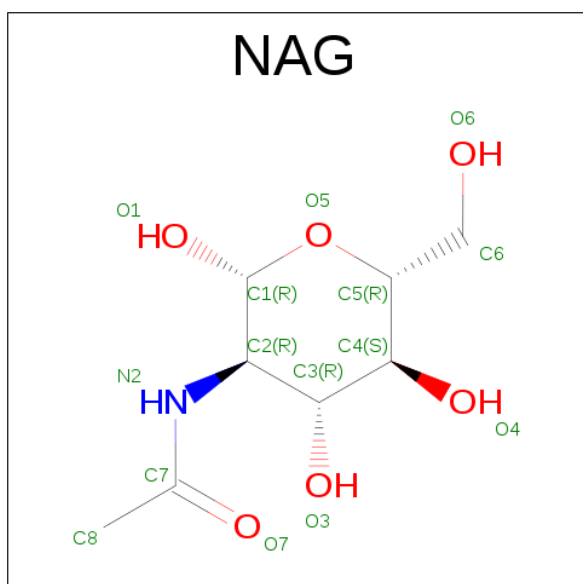
Chain	Residue	Modelled	Actual	Comment	Reference
D	91	GLY	-	EXPRESSION TAG	UNP Q80TS3
D	464	GLY	-	EXPRESSION TAG	UNP Q80TS3
D	465	THR	-	EXPRESSION TAG	UNP Q80TS3
D	466	LYS	-	EXPRESSION TAG	UNP Q80TS3
D	467	HIS	-	EXPRESSION TAG	UNP Q80TS3
D	468	HIS	-	EXPRESSION TAG	UNP Q80TS3
D	469	HIS	-	EXPRESSION TAG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

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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		

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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		

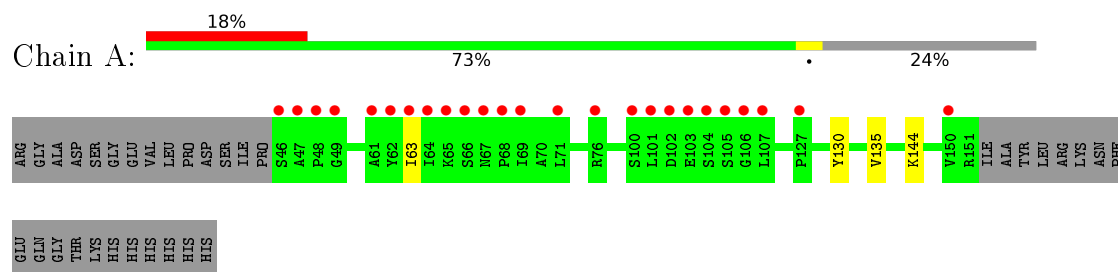
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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		

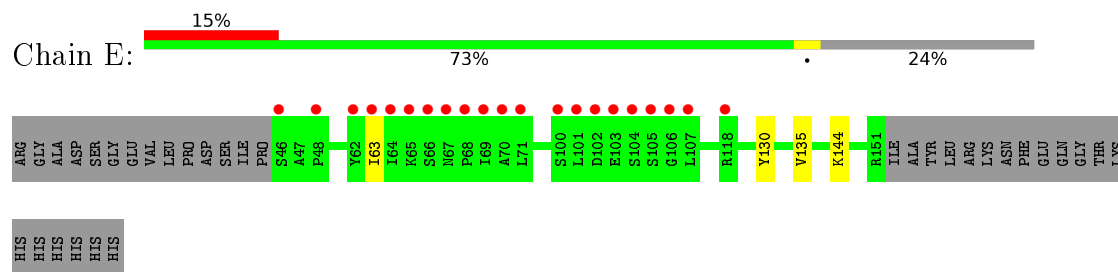
### 3 Residue-property plots [i](#)

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.

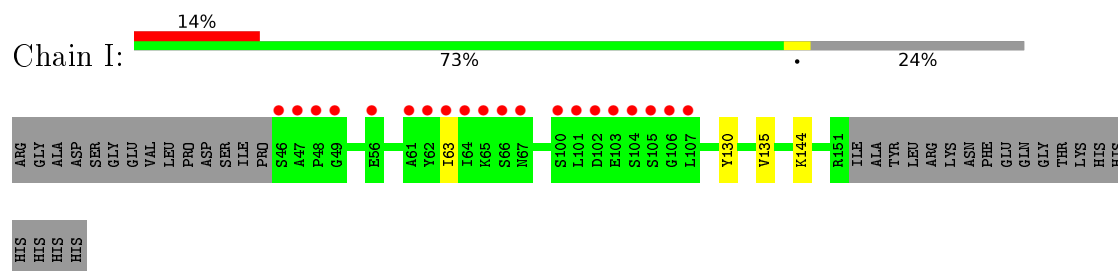
#### • Molecule 1: NETRIN RECEPTOR UNC5D



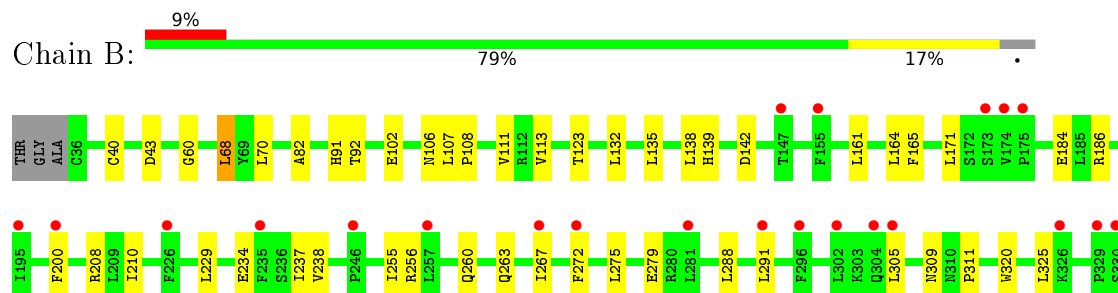
#### • Molecule 1: NETRIN RECEPTOR UNC5D

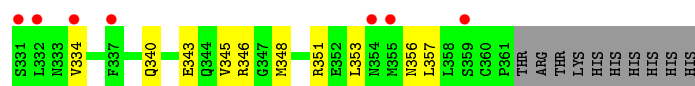


#### • Molecule 1: NETRIN RECEPTOR UNC5D

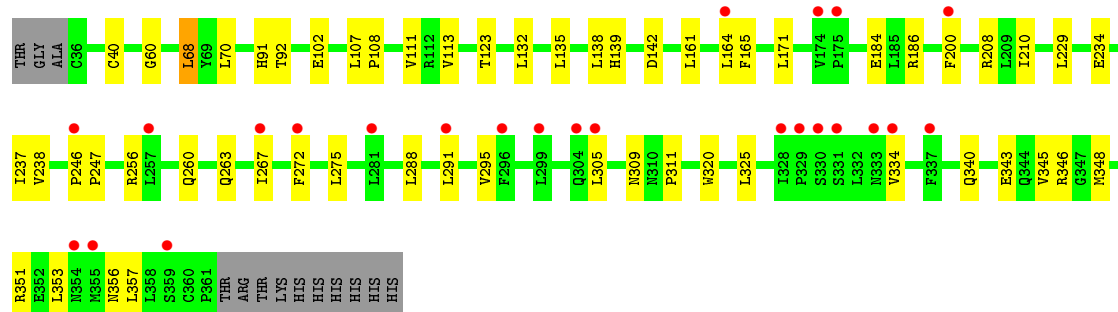
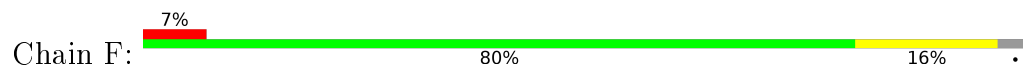


#### • Molecule 2: LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2

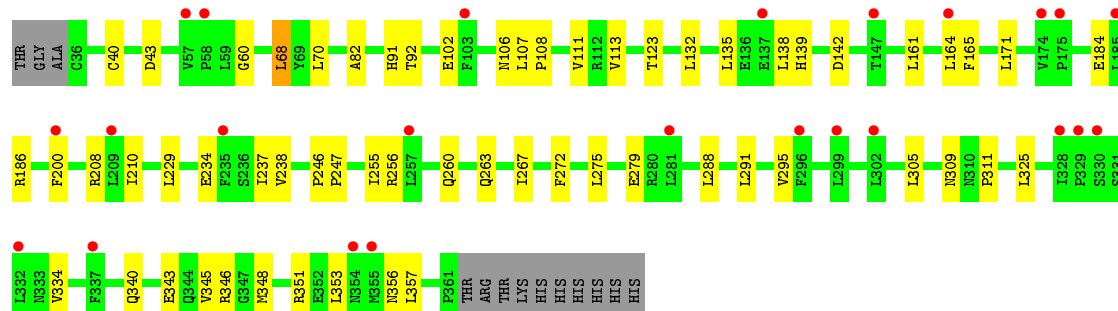
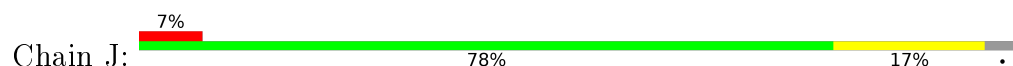




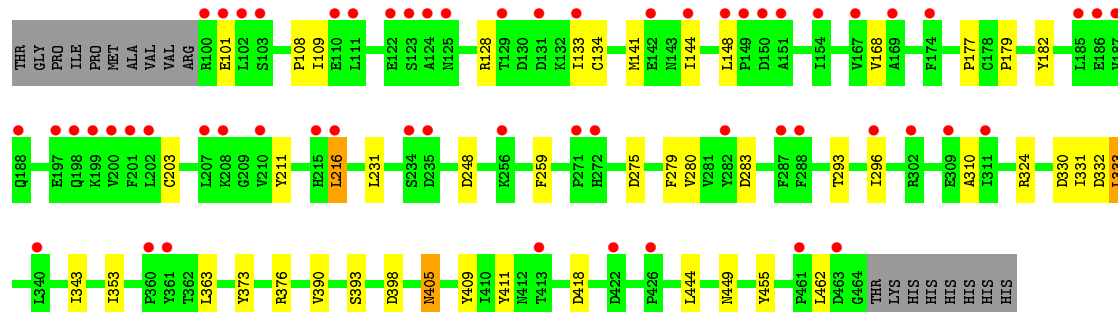
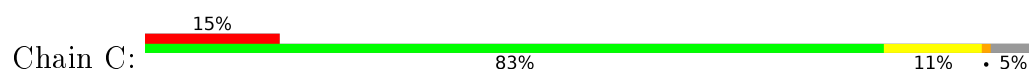
• Molecule 2: LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2



• Molecule 2: LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2

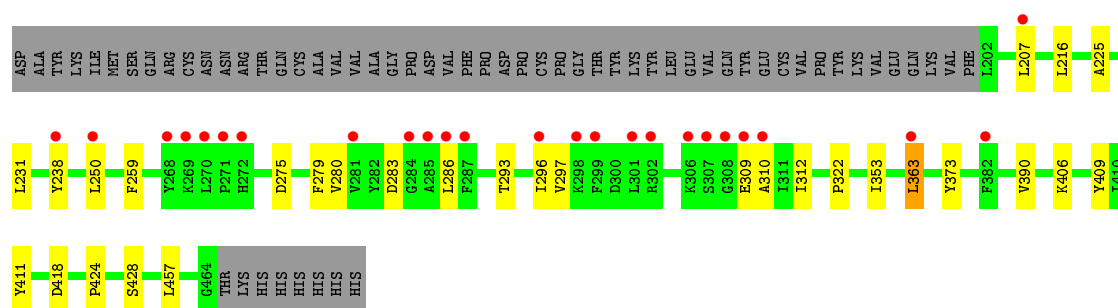


• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3

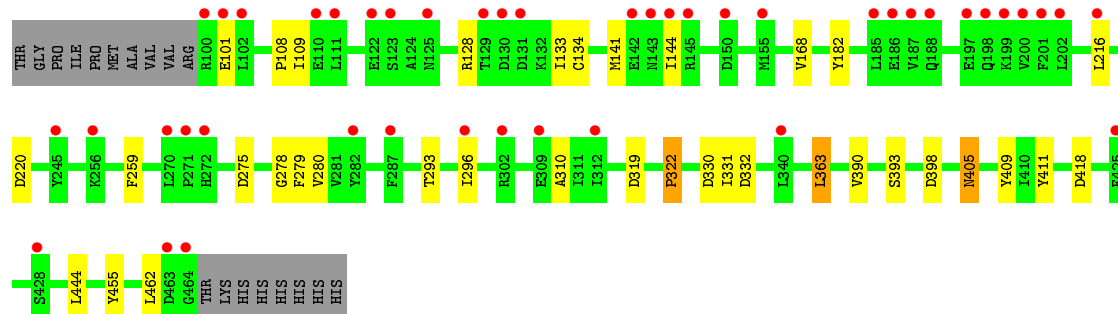
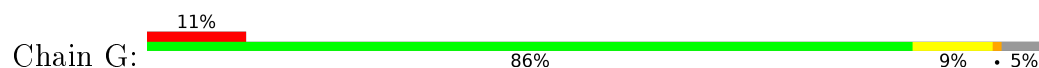


• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3

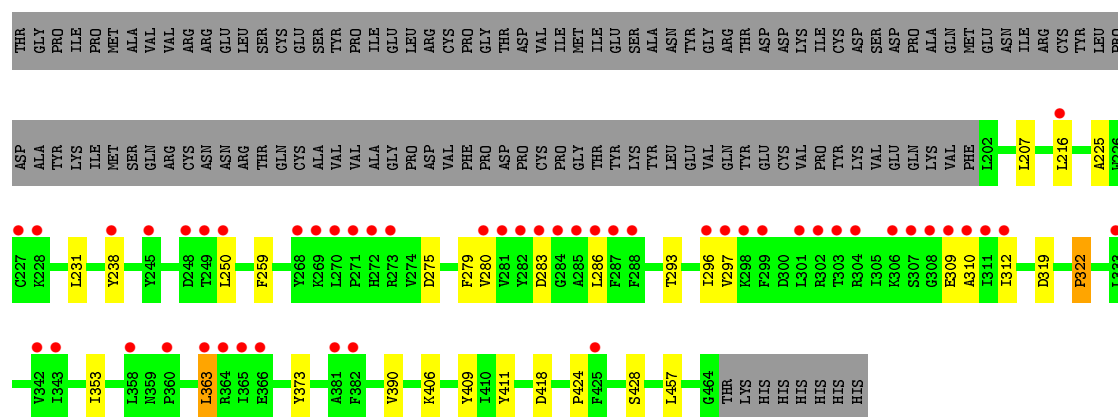




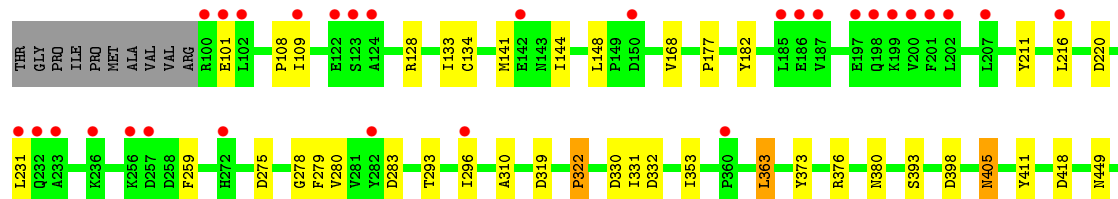
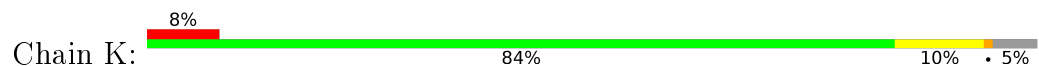
• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3



• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3



• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	344.8	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 316.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.15$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

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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.

All (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

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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
3:G:128:ARG:HH22	3:G:134:CYS:HB2	1.65	0.60
2:F:186:ARG:HH21	2:F:208:ARG:HH12	1.51	0.59
2:J:348:MET:HG2	3:L:428:SER:HB3	1.85	0.58
2:J:186:ARG:HH21	2:J:208:ARG:HH12	1.50	0.58
2:F:234:GLU:HG3	2:F:256:ARG:HB2	1.87	0.57
3:D:225:ALA:HB3	3:D:279:PHE:HD2	1.70	0.56
2:B:186:ARG:HH21	2:B:208:ARG:HH12	1.50	0.56
2:J:234:GLU:HG3	2:J:256:ARG:HB2	1.87	0.56
2:B:234:GLU:HG3	2:B:256:ARG:HB2	1.86	0.56
2:J:184:GLU:HG3	2:J:208:ARG:HB2	1.88	0.56
3:H:225:ALA:HB3	3:H:279:PHE:HD2	1.70	0.55
3:C:310:ALA:HB2	3:C:363:LEU:HB3	1.88	0.55
2:J:107:LEU:HB2	2:J:132:LEU:HD11	1.89	0.55
2:B:107:LEU:HB2	2:B:132:LEU:HD11	1.89	0.54
2:B:238:VAL:HG12	2:B:260:GLN:H	1.73	0.54
2:F:107:LEU:HB2	2:F:132:LEU:HD11	1.89	0.54
3:H:207:LEU:HD11	3:H:457:LEU:HD22	1.90	0.54
2:B:184:GLU:HG3	2:B:208:ARG:HB2	1.88	0.54
2:F:184:GLU:HG3	2:F:208:ARG:HB2	1.88	0.54
2:F:238:VAL:HG12	2:F:260:GLN:H	1.73	0.54
3:L:225:ALA:HB3	3:L:279:PHE:HD2	1.72	0.54
2:J:238:VAL:HG12	2:J:260:GLN:H	1.73	0.53
3:D:207:LEU:HD11	3:D:457:LEU:HD22	1.91	0.53
3:L:207:LEU:HD11	3:L:457:LEU:HD22	1.90	0.52
2:B:305:LEU:HB3	2:B:334:VAL:HG22	1.92	0.52
2:F:305:LEU:HB3	2:F:334:VAL:HG22	1.91	0.52
2:J:305:LEU:HB3	2:J:334:VAL:HG22	1.91	0.52
3:C:216:LEU:HD22	3:C:259:PHE:HD2	1.76	0.51
2:B:353:LEU:HD13	2:B:356:ASN:HA	1.94	0.50
2:F:348:MET:HG2	3:H:428:SER:HB3	1.94	0.50
1:I:135:VAL:HG22	1:I:144:LYS:HG2	1.94	0.49
2:B:161:LEU:HD21	2:B:164:LEU:HD13	1.95	0.49
1:E:135:VAL:HG22	1:E:144:LYS:HG2	1.94	0.49
2:F:353:LEU:HD13	2:F:356:ASN:HA	1.95	0.49
2:J:311:PRO:HA	2:J:340:GLN:HG3	1.95	0.49
3:C:296:ILE:HD11	3:C:331:ILE:HG21	1.93	0.49
2:F:108:PRO:HB2	2:F:111:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG22	1:A:144:LYS:HG2	1.94	0.49
2:B:348:MET:HG2	3:D:428:SER:HB3	1.94	0.48
2:F:200:PHE:HB3	2:F:229:LEU:HD11	1.95	0.48
2:F:68:LEU:HD23	2:F:70:LEU:HD11	1.95	0.48
2:F:311:PRO:HA	2:F:340:GLN:HG3	1.95	0.48
2:B:108:PRO:HB2	2:B:111:VAL:HG23	1.94	0.48
2:J:161:LEU:HD21	2:J:164:LEU:HD13	1.95	0.48
2:B:311:PRO:HA	2:B:340:GLN:HG3	1.95	0.48
2:J:353:LEU:HD13	2:J:356:ASN:HA	1.95	0.48
2:B:200:PHE:HB3	2:B:229:LEU:HD11	1.95	0.48
2:J:68:LEU:HD23	2:J:70:LEU:HD11	1.95	0.48
2:B:68:LEU:HD23	2:B:70:LEU:HD11	1.95	0.48
2:J:200:PHE:HB3	2:J:229:LEU:HD11	1.95	0.48
2:F:161:LEU:HD21	2:F:164:LEU:HD13	1.95	0.47
2:J:108:PRO:HB2	2:J:111:VAL:HG23	1.94	0.47
3:K:310:ALA:HB2	3:K:363:LEU:HB3	1.97	0.46
3:G:101:GLU:HB3	3:G:109:ILE:HD11	1.98	0.46
2:F:135:LEU:HD21	2:F:138:LEU:HD13	1.97	0.46
3:G:310:ALA:HB2	3:G:363:LEU:HB3	1.98	0.46
2:J:135:LEU:HD21	2:J:138:LEU:HD13	1.97	0.46
3:L:411:TYR:HD1	3:L:418:ASP:HB3	1.79	0.46
2:B:135:LEU:HD21	2:B:138:LEU:HD13	1.97	0.45
3:K:101:GLU:HB3	3:K:109:ILE:HD11	1.98	0.45
3:D:411:TYR:HD1	3:D:418:ASP:HB3	1.81	0.45
3:K:278:GLY:HA3	3:K:332:ASP:HA	1.97	0.45
3:L:310:ALA:HB2	3:L:363:LEU:HB3	1.99	0.45
3:G:411:TYR:HD1	3:G:418:ASP:HB3	1.81	0.45
3:H:411:TYR:HD1	3:H:418:ASP:HB3	1.81	0.45
2:J:272:PHE:HA	2:J:275:LEU:HD12	1.99	0.45
3:G:216:LEU:HD22	3:G:259:PHE:HD2	1.82	0.45
3:C:296:ILE:HD12	3:C:333:LEU:HD11	1.99	0.45
3:H:406:LYS:HG2	3:H:424:PRO:HA	1.99	0.45
3:K:319:ASP:HA	3:K:322:PRO:HG3	1.99	0.44
2:J:43:ASP:HB3	3:K:376:ARG:HH22	1.82	0.44
2:B:272:PHE:HA	2:B:275:LEU:HD12	1.98	0.44
3:C:101:GLU:HB3	3:C:109:ILE:HD11	1.98	0.44
3:C:332:ASP:HB3	3:C:343:ILE:HB	1.98	0.44
2:F:272:PHE:HA	2:F:275:LEU:HD12	1.99	0.44
3:G:108:PRO:HB3	3:G:168:VAL:HG22	2.00	0.44
2:J:102:GLU:HG2	2:J:123:THR:HB	2.00	0.44
3:K:216:LEU:HD22	3:K:259:PHE:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:GLU:HA	2:B:346:ARG:HB2	1.99	0.44
3:D:310:ALA:HB2	3:D:363:LEU:HB3	1.98	0.44
3:H:297:VAL:HG22	3:H:309:GLU:HG3	2.00	0.44
3:H:310:ALA:HB2	3:H:363:LEU:HB3	1.99	0.44
2:J:325:LEU:HD22	2:J:351:ARG:HD3	2.00	0.44
2:J:343:GLU:HA	2:J:346:ARG:HB2	1.99	0.43
2:F:325:LEU:HD22	2:F:351:ARG:HD3	2.00	0.43
2:B:325:LEU:HD22	2:B:351:ARG:HD3	2.00	0.43
2:F:343:GLU:HA	2:F:346:ARG:HB2	1.99	0.43
3:K:108:PRO:HB3	3:K:168:VAL:HG22	1.99	0.43
2:J:246:PRO:HA	2:J:247:PRO:HD3	1.93	0.43
3:C:128:ARG:HH21	3:C:182:TYR:HB3	1.82	0.43
2:F:102:GLU:HG2	2:F:123:THR:HB	1.99	0.43
2:F:186:ARG:HE	2:F:210:ILE:HD13	1.84	0.43
2:J:186:ARG:HE	2:J:210:ILE:HD13	1.84	0.43
2:B:102:GLU:HG2	2:B:123:THR:HB	2.00	0.43
2:B:186:ARG:HE	2:B:210:ILE:HD13	1.84	0.43
3:G:278:GLY:HA3	3:G:332:ASP:HA	2.00	0.43
3:C:108:PRO:HB3	3:C:168:VAL:HG22	2.00	0.43
3:D:238:TYR:HB3	3:D:250:LEU:HD11	2.00	0.43
3:L:238:TYR:HB3	3:L:250:LEU:HD11	2.01	0.42
3:K:128:ARG:HH21	3:K:182:TYR:HB3	1.84	0.42
2:J:267:ILE:HD12	2:J:291:LEU:HD21	2.02	0.42
3:K:296:ILE:HD11	3:K:331:ILE:HG21	2.02	0.42
3:L:390:VAL:HB	3:L:409:TYR:HB3	2.01	0.42
3:C:211:TYR:CD1	2:F:320:TRP:HB3	2.55	0.42
3:C:411:TYR:HD1	3:C:418:ASP:HB3	1.84	0.42
3:G:296:ILE:HD11	3:G:331:ILE:HG21	2.01	0.42
3:G:390:VAL:HB	3:G:409:TYR:HB3	2.02	0.42
3:H:238:TYR:HB3	3:H:250:LEU:HD11	2.01	0.42
3:L:250:LEU:HD22	3:L:286:LEU:HD22	2.02	0.42
3:L:296:ILE:HG12	3:L:312:ILE:HD11	2.01	0.42
3:L:297:VAL:HG22	3:L:309:GLU:HG3	2.01	0.42
3:H:296:ILE:HG12	3:H:312:ILE:HD11	2.01	0.42
3:D:297:VAL:HG22	3:D:309:GLU:HG3	2.01	0.42
3:D:231:LEU:HD22	3:D:283:ASP:HB2	2.02	0.42
3:D:296:ILE:HG12	3:D:312:ILE:HD11	2.01	0.42
2:F:92:THR:HG23	2:F:113:VAL:HB	2.02	0.42
3:G:128:ARG:HH21	3:G:182:TYR:HB3	1.84	0.42
3:H:353:ILE:HD12	3:H:373:TYR:HB3	2.02	0.42
3:L:353:ILE:HD12	3:L:373:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:THR:HG23	2:B:113:VAL:HB	2.02	0.41
3:D:250:LEU:HD22	3:D:286:LEU:HD22	2.02	0.41
3:D:216:LEU:HD22	3:D:259:PHE:HD2	1.85	0.41
2:J:91:HIS:HA	2:J:111:VAL:HA	2.03	0.41
3:K:411:TYR:HD1	3:K:418:ASP:HB3	1.85	0.41
2:B:91:HIS:HA	2:B:111:VAL:HA	2.03	0.41
3:C:231:LEU:HD22	3:C:283:ASP:HB2	2.02	0.41
3:C:444:LEU:HB2	3:C:455:TYR:HB2	2.01	0.41
2:J:139:HIS:HA	2:J:165:PHE:HB2	2.02	0.41
3:K:231:LEU:HD22	3:K:283:ASP:HB2	2.02	0.41
3:L:231:LEU:HD22	3:L:283:ASP:HB2	2.02	0.41
3:D:406:LYS:HG2	3:D:424:PRO:HA	2.01	0.41
3:H:250:LEU:HD22	3:H:286:LEU:HD22	2.01	0.41
2:B:267:ILE:HD12	2:B:291:LEU:HD21	2.02	0.41
2:F:267:ILE:HD12	2:F:291:LEU:HD21	2.01	0.41
2:F:91:HIS:HA	2:F:111:VAL:HA	2.03	0.41
2:B:186:ARG:HG3	2:B:210:ILE:HB	2.03	0.41
3:C:148:LEU:HD13	3:C:177:PRO:HG3	2.02	0.41
3:H:319:ASP:HA	3:H:322:PRO:HG3	2.03	0.41
2:B:320:TRP:HB3	3:K:211:TYR:CD1	2.56	0.41
3:L:406:LYS:HG2	3:L:424:PRO:HA	2.03	0.41
3:C:390:VAL:HB	3:C:409:TYR:HB3	2.01	0.41
3:G:444:LEU:HB2	3:G:455:TYR:HB2	2.02	0.41
3:K:148:LEU:HD13	3:K:177:PRO:HG3	2.03	0.41
2:F:139:HIS:HA	2:F:165:PHE:HB2	2.02	0.40
2:J:291:LEU:HD22	2:J:295:VAL:HG11	2.03	0.40
2:J:82:ALA:HA	2:J:106:ASN:HB3	2.03	0.40
2:J:92:THR:HG23	2:J:113:VAL:HB	2.02	0.40
2:B:82:ALA:HA	2:B:106:ASN:HB3	2.03	0.40
3:G:319:ASP:HA	3:G:322:PRO:HG3	2.03	0.40
2:J:255:ILE:HG23	2:J:279:GLU:HB2	2.03	0.40
3:K:353:ILE:HD12	3:K:373:TYR:HB3	2.03	0.40
3:D:353:ILE:HD12	3:D:373:TYR:HB3	2.02	0.40
3:D:390:VAL:HB	3:D:409:TYR:HB3	2.02	0.40
2:F:291:LEU:HD22	2:F:295:VAL:HG11	2.03	0.40
2:F:246:PRO:HA	2:F:247:PRO:HD3	1.93	0.40
3:H:231:LEU:HD22	3:H:283:ASP:HB2	2.03	0.40
3:H:390:VAL:HB	3:H:409:TYR:HB3	2.02	0.40
2:B:139:HIS:HA	2:B:165:PHE:HB2	2.03	0.40
2:B:255:ILE:HG23	2:B:279:GLU:HB2	2.04	0.40
3:C:353:ILE:HD12	3:C:373:TYR:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:ASP:HB3	3:C:376:ARG:HH22	1.85	0.40
3:H:216:LEU:HD22	3:H:259:PHE:HD2	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	248	ASP
3	C	216	LEU

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Mol	Chain	Res	Type
2	B	309	ASN
3	C	449	ASN
2	F	309	ASN
2	J	309	ASN
1	A	130	TYR
1	E	130	TYR
3	K	449	ASN
3	G	133	ILE
1	I	130	TYR
2	B	60	GLY
2	F	60	GLY
2	J	60	GLY
3	K	133	ILE
3	K	322	PRO
3	G	322	PRO
3	L	322	PRO
3	C	133	ILE
3	D	322	PRO
3	H	322	PRO

### 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
2	B	40	CYS
2	B	68	LEU
2	B	142	ASP
2	B	171	LEU
2	B	237	ILE
2	B	263	GLN
2	B	288	LEU
2	B	345	VAL
2	B	357	LEU
3	C	141	MET
3	C	144	ILE
3	C	179	PRO
3	C	203	CYS
3	C	275	ASP
3	C	279	PHE
3	C	280	VAL
3	C	293	THR
3	C	324	ARG
3	C	330	ASP
3	C	333	LEU
3	C	398	ASP
3	C	405	ASN
3	C	462	LEU
3	D	275	ASP
3	D	280	VAL
3	D	293	THR
3	D	363	LEU
1	E	63	ILE
2	F	40	CYS
2	F	68	LEU
2	F	142	ASP
2	F	171	LEU

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Mol	Chain	Res	Type
2	F	237	ILE
2	F	263	GLN
2	F	288	LEU
2	F	345	VAL
2	F	357	LEU
3	G	141	MET
3	G	144	ILE
3	G	220	ASP
3	G	275	ASP
3	G	279	PHE
3	G	280	VAL
3	G	293	THR
3	G	330	ASP
3	G	363	LEU
3	G	398	ASP
3	G	405	ASN
3	G	462	LEU
3	H	275	ASP
3	H	280	VAL
3	H	293	THR
3	H	363	LEU
1	I	63	ILE
2	J	40	CYS
2	J	68	LEU
2	J	142	ASP
2	J	171	LEU
2	J	237	ILE
2	J	263	GLN
2	J	288	LEU
2	J	345	VAL
2	J	357	LEU
3	K	141	MET
3	K	144	ILE
3	K	220	ASP
3	K	275	ASP
3	K	279	PHE
3	K	280	VAL
3	K	293	THR
3	K	330	ASP
3	K	363	LEU
3	K	380	ASN
3	K	398	ASP

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Mol	Chain	Res	Type
3	K	405	ASN
3	K	462	LEU
3	L	275	ASP
3	L	280	VAL
3	L	293	THR
3	L	363	LEU
3	L	380	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
2	B	72	ASN
2	B	310	ASN
2	B	354	ASN
3	C	350	ASN
3	D	212	GLN
3	D	442	ASN
1	E	115	ASN
2	F	72	ASN
2	F	293	GLN
2	F	310	ASN
2	F	354	ASN
3	G	442	ASN
3	H	212	GLN
1	I	80	GLN
1	I	115	ASN
2	J	72	ASN
2	J	293	GLN
2	J	310	ASN
2	J	354	ASN
3	L	212	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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%)
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.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
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
4	F	1362	NAG	C4-C3-C2	-2.41	107.59	111.34
4	C	1465	NAG	C4-C3-C2	-2.22	107.89	111.34
4	G	1465	NAG	C4-C3-C2	-2.21	107.91	111.34
4	K	1465	NAG	C4-C3-C2	-2.20	107.93	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	106/139 (76%)	1.10	25 (23%) <b>1</b> <b>5</b>	162, 191, 238, 249	0
1	E	106/139 (76%)	0.88	21 (19%) <b>1</b> <b>6</b>	162, 191, 238, 249	0
1	I	106/139 (76%)	0.84	20 (18%) <b>2</b> <b>7</b>	162, 191, 238, 249	0
2	B	326/339 (96%)	0.15	29 (8%) <b>12</b> <b>16</b>	127, 162, 226, 250	0
2	F	326/339 (96%)	0.05	24 (7%) <b>17</b> <b>20</b>	127, 162, 226, 250	0
2	J	326/339 (96%)	0.07	24 (7%) <b>17</b> <b>20</b>	127, 162, 226, 250	0
3	C	365/383 (95%)	0.73	58 (15%) <b>3</b> <b>8</b>	112, 152, 257, 274	0
3	D	263/383 (68%)	0.19	25 (9%) <b>10</b> <b>14</b>	187, 227, 271, 278	0
3	G	365/383 (95%)	0.48	44 (12%) <b>6</b> <b>11</b>	112, 152, 257, 274	0
3	H	263/383 (68%)	0.71	50 (19%) <b>2</b> <b>7</b>	187, 227, 271, 278	0
3	K	365/383 (95%)	0.31	30 (8%) <b>14</b> <b>18</b>	112, 152, 257, 274	0
3	L	263/383 (68%)	0.89	56 (21%) <b>1</b> <b>6</b>	187, 227, 271, 278	0
All	All	3180/3732 (85%)	0.44	406 (12%) <b>5</b> <b>10</b>	112, 181, 264, 278	0

All (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
1	A	105	SER	8.4
1	E	105	SER	8.3
3	L	309	GLU	8.2
1	A	102	ASP	8.0
3	C	197	GLU	7.7
3	D	271	PRO	7.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	H	271	PRO	7.3
3	C	200	VAL	7.2
3	K	198	GLN	7.2
3	C	198	GLN	7.1
3	K	200	VAL	7.1
3	G	200	VAL	7.0
3	G	198	GLN	7.0
1	I	104	SER	7.0
3	H	308	GLY	7.0
2	F	354	ASN	6.9
1	A	47	ALA	6.9
1	E	67	ASN	6.7
1	I	105	SER	6.6
3	K	197	GLU	6.6
1	E	66	SER	6.4
1	E	63	ILE	6.3
1	E	68	PRO	6.3
3	D	272	HIS	6.3
3	H	272	HIS	6.2
2	B	175	PRO	6.1
3	L	285	ALA	5.9
1	A	66	SER	5.8
3	H	268	TYR	5.7
3	L	287	PHE	5.7
1	A	67	ASN	5.7
1	A	65	LYS	5.7
3	L	301	LEU	5.6
1	E	65	LYS	5.6
2	B	174	VAL	5.5
1	A	104	SER	5.5
1	I	106	GLY	5.5
3	H	270	LEU	5.4
3	D	269	LYS	5.4
1	E	106	GLY	5.4
3	H	269	LYS	5.4
1	E	69	ILE	5.4
3	L	382	PHE	5.4
3	H	365	ILE	5.3
3	L	269	LYS	5.3
1	I	107	LEU	5.3
2	B	354	ASN	5.2
3	L	281	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
3	C	186	GLU	5.2
2	J	175	PRO	5.2
1	A	46	SER	5.1
3	L	307	SER	5.1
3	L	286	LEU	5.0
3	H	284	GLY	5.0
3	H	286	LEU	5.0
1	I	47	ALA	5.0
3	L	308	GLY	4.9
3	L	227	CYS	4.9
3	L	284	GLY	4.9
3	L	298	LYS	4.9
3	H	285	ALA	4.9
3	K	199	LYS	4.9
1	I	46	SER	4.8
1	A	63	ILE	4.8
3	L	271	PRO	4.8
3	G	142	GLU	4.8
3	K	186	GLU	4.8
1	I	101	LEU	4.8
1	E	104	SER	4.8
1	E	48	PRO	4.7
3	L	238	TYR	4.7
3	L	342	VAL	4.7
3	L	268	TYR	4.6
1	A	106	GLY	4.6
3	C	199	LYS	4.6
1	E	64	ILE	4.6
3	H	287	PHE	4.6
3	L	296	ILE	4.6
3	H	382	PHE	4.6
3	G	122	GLU	4.6
3	G	199	LYS	4.6
3	C	150	ASP	4.6
3	L	299	PHE	4.6
3	L	228	LYS	4.6
3	C	187	VAL	4.5
3	H	307	SER	4.5
3	L	306	LYS	4.5
3	L	310	ALA	4.5
1	E	103	GLU	4.5
1	I	103	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
3	G	272	HIS	4.5
3	L	288	PHE	4.5
2	J	354	ASN	4.4
1	E	101	LEU	4.4
1	I	100	SER	4.4
2	J	174	VAL	4.4
3	K	102	LEU	4.4
3	L	270	LEU	4.3
3	H	238	TYR	4.3
3	G	186	GLU	4.3
1	A	100	SER	4.3
3	C	309	GLU	4.3
3	G	100	ARG	4.3
3	D	270	LEU	4.3
1	I	65	LYS	4.3
3	C	185	LEU	4.3
3	H	381	ALA	4.2
3	L	282	TYR	4.2
3	H	283	ASP	4.2
3	K	122	GLU	4.2
1	E	62	TYR	4.2
3	L	272	HIS	4.1
1	I	67	ASN	4.1
1	I	49	GLY	4.1
3	H	301	LEU	4.1
3	H	363	LEU	4.1
3	H	296	ILE	4.1
3	L	381	ALA	4.1
2	B	296	PHE	4.1
3	C	272	HIS	4.1
3	L	363	LEU	4.1
3	C	122	GLU	4.1
3	D	286	LEU	4.0
3	L	297	VAL	4.0
3	C	463	ASP	4.0
2	J	235	PHE	4.0
3	L	303	THR	4.0
1	I	63	ILE	3.9
3	C	102	LEU	3.9
1	A	101	LEU	3.9
3	D	301	LEU	3.9
3	C	100	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	64	ILE	3.8
1	I	66	SER	3.8
3	G	197	GLU	3.8
3	H	282	TYR	3.8
3	H	281	VAL	3.8
3	L	312	ILE	3.8
3	C	123	SER	3.8
2	F	291	LEU	3.8
3	L	280	VAL	3.8
1	A	107	LEU	3.8
3	K	142	GLU	3.8
1	A	103	GLU	3.7
1	A	68	PRO	3.7
3	K	360	PRO	3.7
3	G	463	ASP	3.7
3	G	201	PHE	3.7
1	E	107	LEU	3.7
3	H	342	VAL	3.7
3	D	309	GLU	3.7
3	H	358	LEU	3.7
3	K	201	PHE	3.7
3	H	306	LYS	3.7
3	L	343	ILE	3.7
3	L	304	ARG	3.6
3	H	298	LYS	3.6
3	D	268	TYR	3.6
3	K	100	ARG	3.6
3	C	142	GLU	3.6
3	G	101	GLU	3.6
2	B	337	PHE	3.6
2	F	337	PHE	3.6
3	L	334	ALA	3.5
3	C	188	GLN	3.5
3	G	102	LEU	3.5
1	I	64	ILE	3.5
2	B	173	SER	3.4
3	K	187	VAL	3.4
3	G	216	LEU	3.4
3	C	282	TYR	3.4
2	F	175	PRO	3.4
1	A	71	LEU	3.4
3	C	461	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
3	H	288	PHE	3.4
3	H	312	ILE	3.3
3	K	185	LEU	3.3
3	H	343	ILE	3.3
3	L	360	PRO	3.3
3	C	287	PHE	3.3
1	A	127	PRO	3.3
3	K	216	LEU	3.3
1	A	69	ILE	3.3
3	C	148	LEU	3.3
3	G	282	TYR	3.3
3	L	389	TYR	3.3
2	F	296	PHE	3.2
3	C	167	VAL	3.2
3	C	101	GLU	3.2
3	H	299	PHE	3.2
2	B	330	SER	3.2
3	K	272	HIS	3.2
3	L	302	ARG	3.2
3	L	207	LEU	3.2
2	F	355	MET	3.2
1	E	100	SER	3.1
2	B	246	PRO	3.1
2	B	355	MET	3.1
3	D	306	LYS	3.1
3	K	150	ASP	3.1
3	H	303	THR	3.1
3	G	144	ILE	3.1
2	F	174	VAL	3.1
1	A	61	ALA	3.1
2	B	334	VAL	3.1
3	G	271	PRO	3.1
3	L	300	ASP	3.0
3	D	296	ILE	3.0
2	J	164	LEU	3.0
3	G	145	ARG	3.0
3	G	150	ASP	3.0
2	B	155	PHE	3.0
2	J	296	PHE	3.0
3	C	207	LEU	3.0
3	G	464	GLY	3.0
3	H	280	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	329	PRO	3.0
2	B	291	LEU	2.9
3	G	123	SER	2.9
2	J	257	LEU	2.9
3	G	155	MET	2.9
3	C	111	LEU	2.9
2	F	257	LEU	2.9
3	K	282	TYR	2.9
2	B	305	LEU	2.9
3	K	256	LYS	2.9
3	G	202	LEU	2.9
1	E	71	LEU	2.9
2	F	304	GLN	2.9
3	C	154	ILE	2.9
3	C	360	PRO	2.9
3	D	250	LEU	2.8
3	D	308	GLY	2.8
3	D	310	ALA	2.8
3	D	382	PHE	2.8
2	J	185	LEU	2.8
3	C	296	ILE	2.8
3	H	310	ALA	2.8
3	C	201	PHE	2.8
2	B	326	LYS	2.8
3	G	143	ASN	2.8
3	G	312	ILE	2.8
3	K	101	GLU	2.7
3	L	283	ASP	2.7
3	G	287	PHE	2.7
3	D	207	LEU	2.7
3	D	299	PHE	2.7
3	G	425	PHE	2.7
2	J	355	MET	2.7
3	L	361	TYR	2.7
3	C	174	PHE	2.7
2	B	329	PRO	2.7
3	C	110	GLU	2.7
3	C	271	PRO	2.7
3	G	256	LYS	2.7
1	E	70	ALA	2.7
3	C	216	LEU	2.7
3	L	335	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	G	131	ASP	2.6
2	B	332	LEU	2.6
3	C	124	ALA	2.6
3	D	298	LYS	2.6
3	H	311	ILE	2.6
2	J	302	LEU	2.6
3	L	358	LEU	2.6
3	C	169	ALA	2.6
3	G	309	GLU	2.6
2	B	281	LEU	2.6
2	B	304	GLN	2.6
2	B	147	THR	2.6
3	C	422	ASP	2.5
3	G	340	LEU	2.5
3	C	235	ASP	2.5
2	B	257	LEU	2.5
3	H	249	THR	2.5
3	K	202	LEU	2.5
3	H	364	ARG	2.5
2	F	330	SER	2.5
3	D	307	SER	2.5
3	C	215	HIS	2.5
2	J	329	PRO	2.5
3	C	149	PRO	2.5
3	K	123	SER	2.5
3	H	302	ARG	2.4
2	B	226	PHE	2.4
3	C	413	THR	2.4
2	J	209	LEU	2.4
3	C	103	SER	2.4
2	J	137	GLU	2.4
3	L	435	VAL	2.4
3	C	426	PRO	2.4
3	G	296	ILE	2.4
2	B	302	LEU	2.4
3	L	333	LEU	2.4
1	A	62	TYR	2.4
3	C	133	ILE	2.4
3	L	292	ARG	2.4
3	H	216	LEU	2.4
2	F	299	LEU	2.4
3	G	428	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	304	ARG	2.4
3	L	313	ALA	2.4
3	H	250	LEU	2.4
3	G	129	THR	2.4
3	H	227	CYS	2.4
3	L	362	THR	2.4
3	L	226	TRP	2.4
2	B	331	SER	2.4
2	J	332	LEU	2.4
3	G	110	GLU	2.4
3	G	270	LEU	2.4
2	F	272	PHE	2.3
3	G	111	LEU	2.3
3	D	281	VAL	2.3
2	F	305	LEU	2.3
2	J	281	LEU	2.3
2	F	267	ILE	2.3
3	C	125	ASN	2.3
3	G	130	ASP	2.3
3	K	124	ALA	2.3
2	B	200	PHE	2.3
3	H	228	LYS	2.3
3	C	340	LEU	2.3
3	D	302	ARG	2.3
1	I	62	TYR	2.3
3	C	234	SER	2.3
2	B	272	PHE	2.3
3	D	363	LEU	2.3
2	F	331	SER	2.3
3	C	361	TYR	2.3
1	A	49	GLY	2.3
1	E	46	SER	2.3
2	F	281	LEU	2.3
2	J	299	LEU	2.3
3	H	360	PRO	2.3
2	J	337	PHE	2.3
3	H	248	ASP	2.3
3	D	238	TYR	2.3
3	H	333	LEU	2.3
2	B	235	PHE	2.3
3	D	284	GLY	2.2
3	H	425	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	267	ILE	2.2
3	H	245	TYR	2.2
2	F	164	LEU	2.2
3	K	109	ILE	2.2
3	D	285	ALA	2.2
3	K	296	ILE	2.2
2	F	334	VAL	2.2
1	I	56	GLU	2.2
3	K	232	GLN	2.2
2	J	58	PRO	2.2
3	K	257	ASP	2.2
3	C	256	LYS	2.2
1	E	118	ARG	2.2
3	C	144	ILE	2.2
2	F	359	SER	2.2
1	I	61	ALA	2.2
3	G	188	GLN	2.2
3	L	311	ILE	2.2
3	C	151	ALA	2.2
3	G	245	TYR	2.2
2	B	359	SER	2.2
3	G	185	LEU	2.2
2	F	328	ILE	2.2
3	L	364	ARG	2.2
3	G	302	ARG	2.2
3	L	444	LEU	2.1
3	C	202	LEU	2.1
3	C	208	LYS	2.1
2	F	246	PRO	2.1
3	C	129	THR	2.1
3	C	131	ASP	2.1
3	K	233	ALA	2.1
1	A	76	ARG	2.1
2	B	195	ILE	2.1
3	D	287	PHE	2.1
3	C	210	VAL	2.1
1	A	150	VAL	2.1
3	C	302	ARG	2.1
3	H	366	GLU	2.1
2	F	333	ASN	2.1
2	J	147	THR	2.1
3	H	297	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	330	SER	2.1
3	C	311	ILE	2.1
3	H	273	ARG	2.1
3	L	383	MET	2.1
3	L	436	ASP	2.1
3	K	207	LEU	2.0
2	J	328	ILE	2.0
2	J	57	VAL	2.0
3	K	231	LEU	2.0
2	F	200	PHE	2.0
3	L	425	PHE	2.0
3	G	125	ASN	2.0
3	K	236	LYS	2.0
2	J	103	PHE	2.0
2	J	200	PHE	2.0
3	C	288	PHE	2.0
3	G	187	VAL	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<sup>th</sup> 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( $\text{\AA}^2$ )	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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 [i](#)

There are no such residues in this entry.