Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 07:00 am GMT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

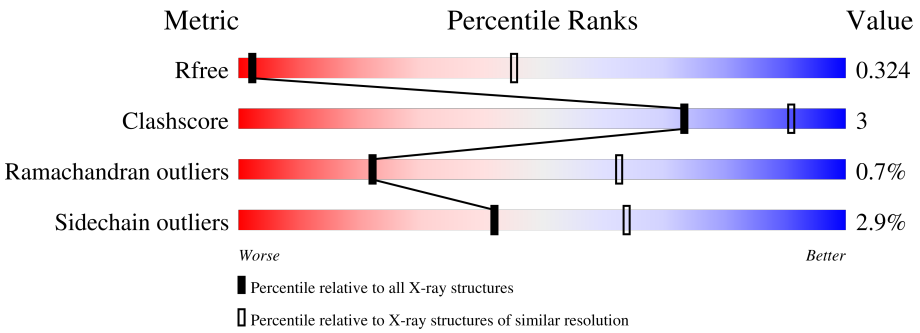
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1018 (8.20-3.82)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	139	73% • 24%
1	E	139	73% • 24%
1	I	139	73% • 24%
2	B	339	79% 17% •
2	F	339	80% 16% •
2	J	339	78% 17% •
3	C	383	83% 11% • 5%

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Mol	Chain	Length	Quality of chain
3	D	383	61% 8% 31%
3	G	383	86% 9% • 5%
3	H	383	61% 8% • 31%
3	K	383	84% 10% • 5%
3	L	383	61% 7% 31%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	106	853	536	152	160	5	0	0	0
1	E	106	853	536	152	160	5	0	0	0
1	I	106	853	536	152	160	5	0	0	0

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
			Total	C	N	O	S			
2	B	326	2587	1634	461	478	14	0	0	0
2	F	326	2587	1634	461	478	14	0	0	0
2	J	326	2587	1634	461	478	14	0	0	0

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
			Total	C	N	O	S			
3	C	365	2943	1867	485	575	16	0	0	0
			Total	C	N	O	S			
3	D	263	2131	1360	351	415	5	0	0	0
			Total	C	N	O	S			
3	G	365	2943	1867	485	575	16	0	0	0
			Total	C	N	O	S			
3	H	263	2131	1360	351	415	5	0	0	0
			Total	C	N	O	S			
3	K	365	2943	1867	485	575	16	0	0	0
			Total	C	N	O	S			
3	L	263	2131	1360	351	415	5	0	0	0

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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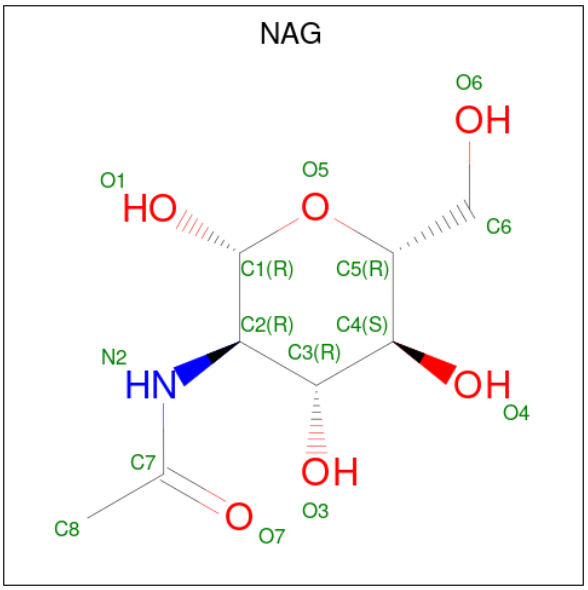
Chain	Residue	Modelled	Actual	Comment	Reference
K	472	HIS	-	expression tag	UNP Q80TS3
L	90	THR	-	expression tag	UNP Q80TS3
L	91	GLY	-	expression tag	UNP Q80TS3
L	464	GLY	-	expression tag	UNP Q80TS3
L	465	THR	-	expression tag	UNP Q80TS3
L	466	LYS	-	expression tag	UNP Q80TS3
L	467	HIS	-	expression tag	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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	14	0
			Total	C	N	O		
4	C	1	14	8	1	5	14	0
			Total	C	N	O		
4	E	1	14	8	1	5	0	0
			Total	C	N	O		
4	F	1	14	8	1	5	14	0

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

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

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

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

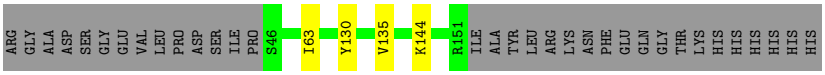
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	C	1	1	1	0	0
6	D	1	1	1	0	0
6	G	1	1	1	0	0
6	H	1	1	1	0	0
6	K	1	1	1	0	0
6	L	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

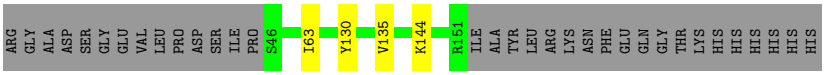
• Molecule 1: NETRIN RECEPTOR UNC5D

Chain A:



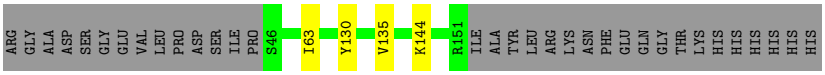
• Molecule 1: NETRIN RECEPTOR UNC5D

Chain E:



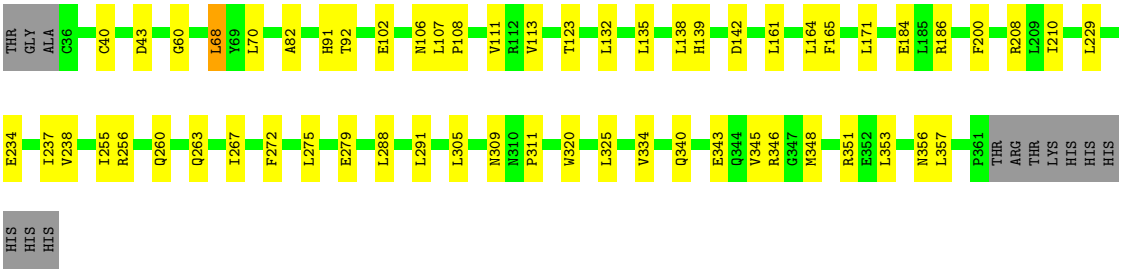
• Molecule 1: NETRIN RECEPTOR UNC5D

Chain I:



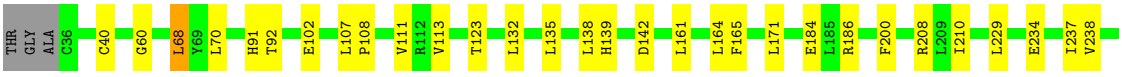
• Molecule 2: LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2

Chain B:



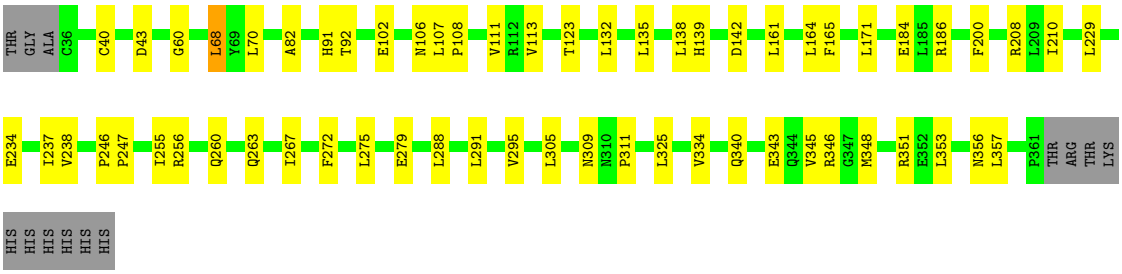
• Molecule 2: LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2

Chain F:



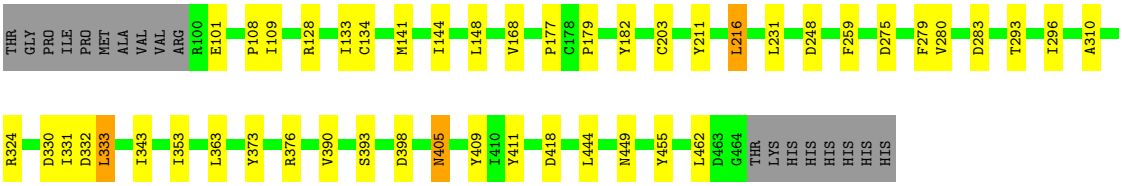
• Molecule 2: LEUCINE-RICH REPEAT TRANSMEMBRANE PROTEIN FLRT2

Chain J:



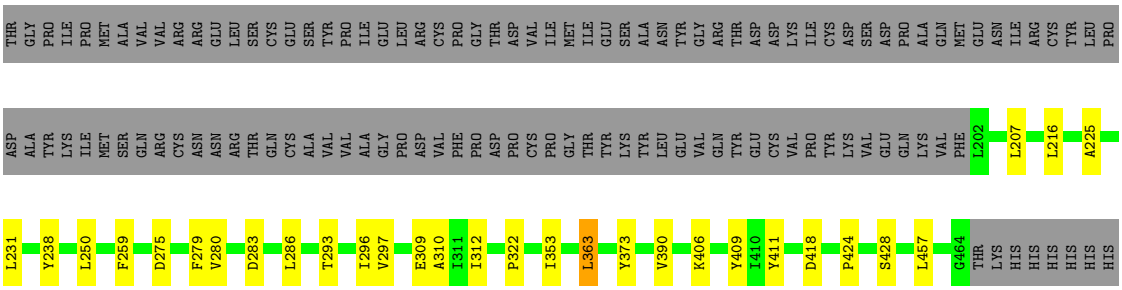
• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3

Chain C:



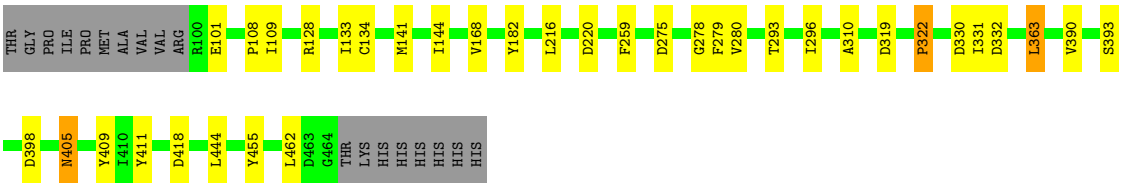
• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3

Chain D:



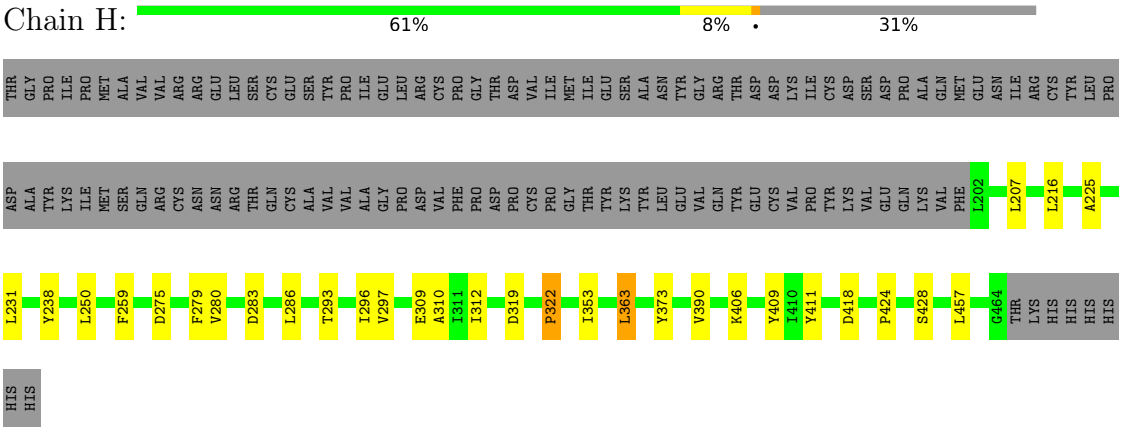
• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3

Chain G:



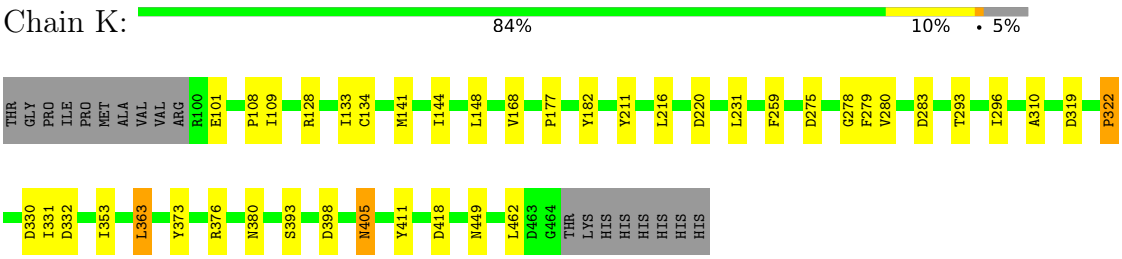
• Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3

Chain H:



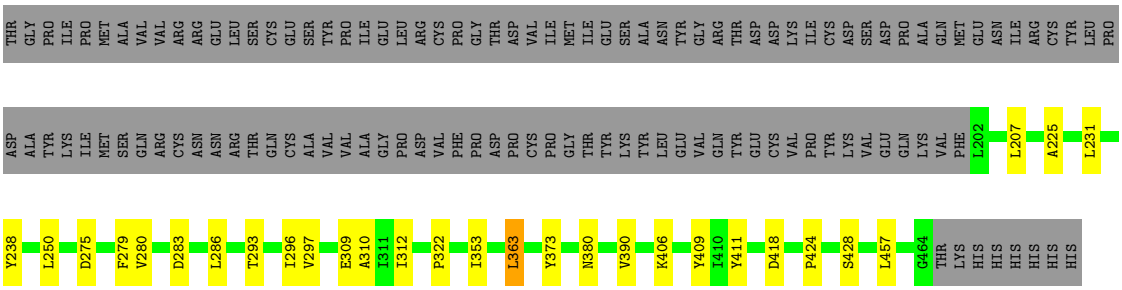
- Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3

Chain K:



- Molecule 3: ADHESION G PROTEIN-COUPLED RECEPTOR L3

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	292.36Å 292.36Å 291.77Å 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
$< I/\sigma(I) >$ [1]	1.43 (at 6.20Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.276 , 0.278 0.330 , 0.324	Depositor DCC
R_{free} test set	719 reflections (4.55%)	wwPDB-VP
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]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, NAG, CA

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:68:LEU:HD23	2:F:70:LEU:HD11	1.95	0.48
2:F:200:PHE:HB3	2:F:229: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:91:HIS:HA	2:F:111:VAL:HA	2.03	0.41
2:F:267:ILE:HD12	2:F:291:LEU:HD21	2.01	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
2:B:320:TRP:HB3	3:K:211:TYR:CD1	2.56	0.41
3:C:390:VAL:HB	3:C:409:TYR:HB3	2.01	0.41
3:H:319:ASP:HA	3:H:322:PRO:HG3	2.03	0.41
3:L:406:LYS:HG2	3:L:424:PRO:HA	2.03	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: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:J:291:LEU:HD22	2:J:295:VAL:HG11	2.03	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:43:ASP:HB3	3:C:376:ARG:HH22	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:353:ILE:HD12	3:C:373:TYR:HB3	2.02	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%)	15	54
1	E	104/139 (75%)	101 (97%)	2 (2%)	1 (1%)	15	54
1	I	104/139 (75%)	101 (97%)	2 (2%)	1 (1%)	15	54
2	B	322/339 (95%)	285 (88%)	35 (11%)	2 (1%)	25	66
2	F	322/339 (95%)	285 (88%)	35 (11%)	2 (1%)	25	66
2	J	322/339 (95%)	285 (88%)	35 (11%)	2 (1%)	25	66
3	C	363/383 (95%)	330 (91%)	29 (8%)	4 (1%)	14	52
3	D	259/383 (68%)	241 (93%)	17 (7%)	1 (0%)	34	72
3	G	363/383 (95%)	334 (92%)	27 (7%)	2 (1%)	25	66
3	H	259/383 (68%)	241 (93%)	17 (7%)	1 (0%)	34	72
3	K	363/383 (95%)	334 (92%)	26 (7%)	3 (1%)	19	60
3	L	259/383 (68%)	241 (93%)	17 (7%)	1 (0%)	34	72
All	All	3144/3732 (84%)	2879 (92%)	244 (8%)	21 (1%)	22	62

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 (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	94/122 (77%)	93 (99%)	1 (1%)	73	84
1	E	94/122 (77%)	93 (99%)	1 (1%)	73	84
1	I	94/122 (77%)	93 (99%)	1 (1%)	73	84
2	B	297/308 (96%)	288 (97%)	9 (3%)	41	63
2	F	297/308 (96%)	288 (97%)	9 (3%)	41	63
2	J	297/308 (96%)	288 (97%)	9 (3%)	41	63
3	C	324/340 (95%)	310 (96%)	14 (4%)	29	54
3	D	231/340 (68%)	227 (98%)	4 (2%)	60	78
3	G	324/340 (95%)	312 (96%)	12 (4%)	34	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	231/340 (68%)	227 (98%)	4 (2%)	60	78
3	K	324/340 (95%)	311 (96%)	13 (4%)	31	55
3	L	231/340 (68%)	226 (98%)	5 (2%)	52	71
All	All	2838/3330 (85%)	2756 (97%)	82 (3%)	42	64

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

Sometimes 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 (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 monosaccharides 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	J	1362	-	14,14,15	0.46	0	17,19,21	1.13	2 (11%)
4	NAG	I	1152	-	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
4	NAG	C	1465	-	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
4	NAG	F	1362	-	14,14,15	0.45	0	17,19,21	1.13	2 (11%)
4	NAG	E	1152	-	14,14,15	0.44	0	17,19,21	1.15	2 (11%)
4	NAG	B	1362	-	14,14,15	0.45	0	17,19,21	1.14	2 (11%)
4	NAG	A	1152	-	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
4	NAG	K	1465	-	14,14,15	0.54	0	17,19,21	0.91	1 (5%)
4	NAG	G	1465	-	14,14,15	0.55	0	17,19,21	0.92	1 (5%)

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	J	1362	-	-	0/6/23/26	0/1/1/1
4	NAG	I	1152	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1465	-	-	3/6/23/26	0/1/1/1
4	NAG	F	1362	-	-	0/6/23/26	0/1/1/1
4	NAG	E	1152	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1362	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1152	-	-	0/6/23/26	0/1/1/1
4	NAG	K	1465	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1465	-	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1152	NAG	C4-C3-C2	-2.44	107.44	111.02
4	E	1152	NAG	C4-C3-C2	-2.43	107.46	111.02
4	A	1152	NAG	C4-C3-C2	-2.41	107.48	111.02
4	J	1362	NAG	C4-C3-C2	-2.36	107.56	111.02
4	B	1362	NAG	C4-C3-C2	-2.35	107.58	111.02
4	F	1362	NAG	C4-C3-C2	-2.34	107.59	111.02
4	B	1362	NAG	C8-C7-N2	2.14	119.72	116.10
4	C	1465	NAG	C4-C3-C2	-2.14	107.89	111.02
4	J	1362	NAG	C8-C7-N2	2.13	119.70	116.10
4	G	1465	NAG	C4-C3-C2	-2.12	107.91	111.02
4	A	1152	NAG	C8-C7-N2	2.12	119.69	116.10
4	I	1152	NAG	C8-C7-N2	2.11	119.67	116.10
4	K	1465	NAG	C4-C3-C2	-2.11	107.93	111.02
4	F	1362	NAG	C8-C7-N2	2.10	119.66	116.10
4	E	1152	NAG	C8-C7-N2	2.08	119.63	116.10

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1465	NAG	C4-C5-C6-O6
4	G	1465	NAG	C4-C5-C6-O6
4	K	1465	NAG	C4-C5-C6-O6
4	K	1465	NAG	O5-C5-C6-O6
4	C	1465	NAG	O5-C5-C6-O6
4	G	1465	NAG	O5-C5-C6-O6
4	C	1465	NAG	C3-C2-N2-C7
4	G	1465	NAG	C3-C2-N2-C7
4	K	1465	NAG	C3-C2-N2-C7

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	F	1
3	H	1
2	J	1
3	L	1
3	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	307:ALA	C	308:ARG	N	3.26
1	F	307:ALA	C	308:ARG	N	3.26
1	H	295:ASN	C	296:ILE	N	3.25
1	J	307:ALA	C	308:ARG	N	3.25
1	L	295:ASN	C	296:ILE	N	3.25
1	D	295:ASN	C	296:ILE	N	3.24

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.