Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2MUS
BMRB ID	:	11064
Title	:	HADDOCK calculated model of LIN5001 bound to the HET-s amyloid
Authors	:	Hermann, U.S.; Schuetz, A.K.; Shirani, H.; Saban, D.; Nuvolone, M.; Huang, D.H.; Li, B.; Ballmer, B.; Aslund, A.K.O.; Mason, J.J.; Rushing, E.; Budka, H.; Hammarstrom, P.; Bockmann, A.; Caflisch, A.; Meier, B.H.; Nilsson, P.K.R.; Hornemann, S.; Aguzzi, A.
Deposited on	:	2014-09-16

This is a Full wwPDB NMR 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/NMRValidationReportHelp
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:

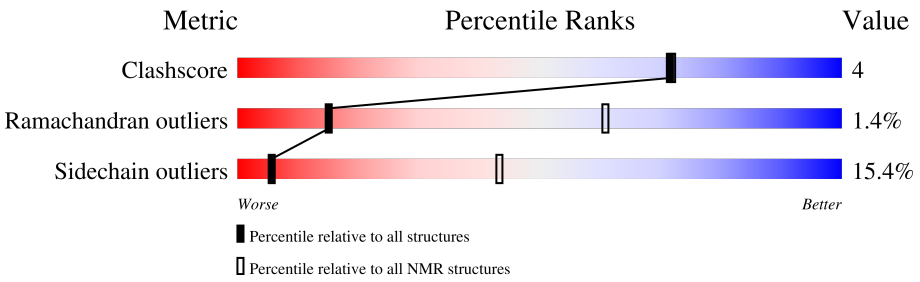
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 6%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	79	85% 5% 10%
1	B	79	82% 8% 10%
1	C	79	76% 14% 10%
1	D	79	78% 11% 10%
1	E	79	75% 14% • 10%

2 Ensemble composition and analysis (i)

This entry contains 4 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:225-A:295, B:225-B:295, C:225-C:295, D:225-D:295, E:225-E:295 (355)	0.45	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5496 atoms, of which 2692 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heterokaryon incompatibility protein s.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	71	1089	335	536	115	103	0
1	B	71	1089	335	536	115	103	0
1	C	71	1089	335	536	115	103	0
1	D	71	1089	335	536	115	103	0
1	E	71	1089	335	536	115	103	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	MET	-	initiating methionine	UNP Q03689
A	265	LYS	GLU	conflict	UNP Q03689
A	290	HIS	-	expression tag	UNP Q03689
A	291	HIS	-	expression tag	UNP Q03689
A	292	HIS	-	expression tag	UNP Q03689
A	293	HIS	-	expression tag	UNP Q03689
A	294	HIS	-	expression tag	UNP Q03689
A	295	HIS	-	expression tag	UNP Q03689
B	217	MET	-	initiating methionine	UNP Q03689
B	265	LYS	GLU	conflict	UNP Q03689
B	290	HIS	-	expression tag	UNP Q03689
B	291	HIS	-	expression tag	UNP Q03689
B	292	HIS	-	expression tag	UNP Q03689
B	293	HIS	-	expression tag	UNP Q03689
B	294	HIS	-	expression tag	UNP Q03689
B	295	HIS	-	expression tag	UNP Q03689
C	217	MET	-	initiating methionine	UNP Q03689
C	265	LYS	GLU	conflict	UNP Q03689
C	290	HIS	-	expression tag	UNP Q03689
C	291	HIS	-	expression tag	UNP Q03689
C	292	HIS	-	expression tag	UNP Q03689
C	293	HIS	-	expression tag	UNP Q03689
C	294	HIS	-	expression tag	UNP Q03689

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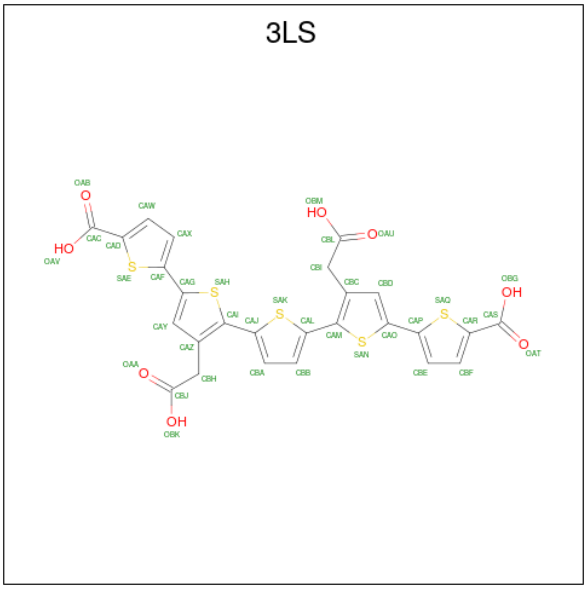
Chain	Residue	Modelled	Actual	Comment	Reference
C	295	HIS	-	expression tag	UNP Q03689
D	217	MET	-	initiating methionine	UNP Q03689
D	265	LYS	GLU	conflict	UNP Q03689
D	290	HIS	-	expression tag	UNP Q03689
D	291	HIS	-	expression tag	UNP Q03689
D	292	HIS	-	expression tag	UNP Q03689
D	293	HIS	-	expression tag	UNP Q03689
D	294	HIS	-	expression tag	UNP Q03689
D	295	HIS	-	expression tag	UNP Q03689
E	217	MET	-	initiating methionine	UNP Q03689
E	265	LYS	GLU	conflict	UNP Q03689
E	290	HIS	-	expression tag	UNP Q03689
E	291	HIS	-	expression tag	UNP Q03689
E	292	HIS	-	expression tag	UNP Q03689
E	293	HIS	-	expression tag	UNP Q03689
E	294	HIS	-	expression tag	UNP Q03689
E	295	HIS	-	expression tag	UNP Q03689

- Molecule 2 is 3’’’,4’-bis(carboxymethyl)-2,2’:5’,2’’:5’’,2’’’:5’’’,2’’’’-quinquethiophene-5,5’’’’-di carboxylic acid (three-letter code: 3LS) (formula: $C_{26}H_{16}O_8S_5$).



Mol	Chain	Residues	Atoms				
			Total	C	H	O	S
2	B	1	51	26	12	8	5

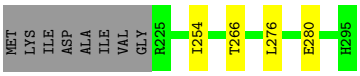
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Heterokaryon incompatibility protein s

Chain A:



• Molecule 1: Heterokaryon incompatibility protein s

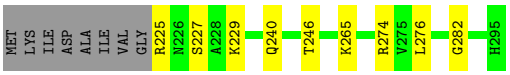
Chain B:

• Molecule 1: Heterokaryon incompatibility protein s

Chain C:

• Molecule 1: Heterokaryon incompatibility protein s

Chain D:



• Molecule 1: Heterokaryon incompatibility protein s

Chain E:

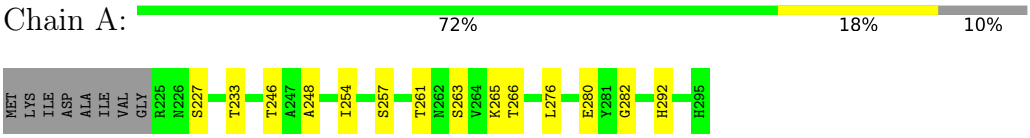
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

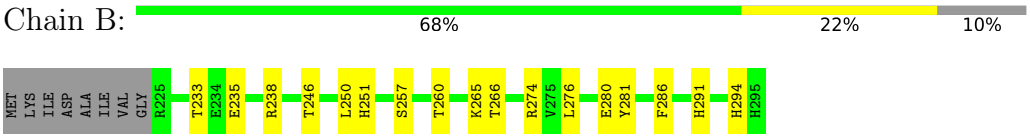
• Molecule 1: Heterokaryon incompatibility protein s

Chain A:



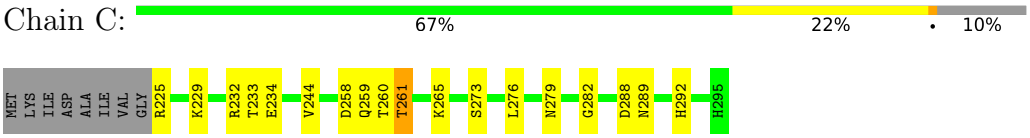
• Molecule 1: Heterokaryon incompatibility protein s

Chain B:



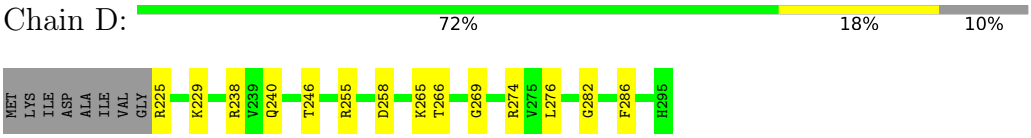
• Molecule 1: Heterokaryon incompatibility protein s

Chain C:



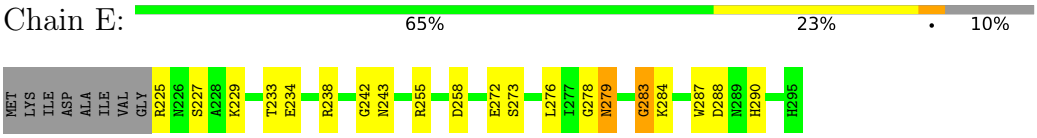
• Molecule 1: Heterokaryon incompatibility protein s

Chain D:



• Molecule 1: Heterokaryon incompatibility protein s

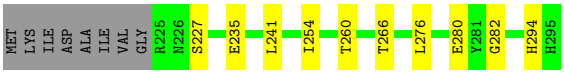
Chain E:



4.2.2 Score per residue for model 2

• Molecule 1: Heterokaryon incompatibility protein s

Chain A:

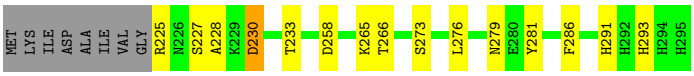


• Molecule 1: Heterokaryon incompatibility protein s

Chain B:

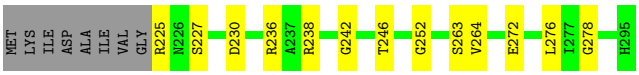
• Molecule 1: Heterokaryon incompatibility protein s

Chain C:



• Molecule 1: Heterokaryon incompatibility protein s

Chain D:



• Molecule 1: Heterokaryon incompatibility protein s

Chain E:

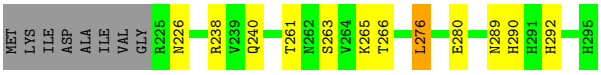
4.2.3 Score per residue for model 3

• Molecule 1: Heterokaryon incompatibility protein s

Chain A:

• Molecule 1: Heterokaryon incompatibility protein s

Chain B:



• Molecule 1: Heterokaryon incompatibility protein s

Chain C: 70% 16% • 10%

MET LYS ILE ASP ALA ILE VAL GLY R225 T233 R238 L241 D258 T261 N262 S263 T266 S273 R274 V275 L276 I277 Y281 G282 G283 W287 D288 H293 H294 H295

• Molecule 1: Heterokaryon incompatibility protein s

Chain D: 68% 22% 10%

MET LYS ILE ASP ALA ILE VAL GLY R225 N226 S227 A228 K229 T233 R236 Q240 T246 D258 N262 K265 E272 S273 R274 V275 L276 Y281 G282 W287 D288 H295

• Molecule 1: Heterokaryon incompatibility protein s

Chain E: 71% 18% • 10%

MET LYS ILE ASP ALA ILE VAL GLY R225 N226 K229 R238 R255 T261 K265 K270 S273 R274 V275 L276 E280 G283 W287 H290 H295

4.2.4 Score per residue for model 4

• Molecule 1: Heterokaryon incompatibility protein s

Chain A: 77% 13% 10%

MET LYS ILE ASP ALA ILE VAL GLY R225 D230 I254 R255 T260 K265 T266 S273 L276 E280 G283 H295

• Molecule 1: Heterokaryon incompatibility protein s

Chain B: 72% 18% 10%

MET LYS ILE ASP ALA ILE VAL GLY R225 T233 R238 H251 T260 S263 T266 G269 S273 L276 E280 N289 H290 H291 H292 H295

• Molecule 1: Heterokaryon incompatibility protein s

Chain C: 71% 15% • 10%

MET LYS ILE ASP ALA ILE VAL GLY R225 D230 T233 R238 S257 D258 Q259 T260 T261 S273 R274 V275 L276 Y281 W287 D288 H291 H292 H295

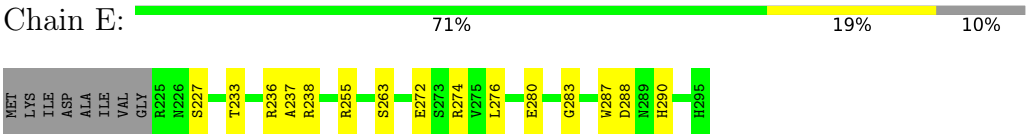
• Molecule 1: Heterokaryon incompatibility protein s

Chain D: 75% 13% • 10%

MET LYS ILE ASP ALA ILE VAL GLY R225 N226 S227 A228 K229 Q240 V245 T246 Q259 S263 V264 K265 R274 G282 F286 H295

• Molecule 1: Heterokaryon incompatibility protein s

Chain E:


71%
19%
10%
MET
LYS
ILE
ASP
ALA
ILE
VAL
GLY
R225
N226
S227
T233
R236
A237
R238
R255
S263
E272
S273
R274
V275
L276
E280
G283
W287
D288
N289
H290
H295

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 200 calculated structures, 4 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	structure solution	
HADDOCK	geometry optimization	
HADDOCK	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	320
Number of shifts mapped to atoms	304
Number of unparsed shifts	0
Number of shifts with mapping errors	16
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	6%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3LS

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	553	536	535	2±1
1	B	553	536	535	4±1
1	C	553	536	535	6±3
1	D	553	536	535	6±2
1	E	553	536	535	4±1
2	B	39	12	0	5±1
All	All	11216	10768	10700	77

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 4.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:301:3LS:SAK	2:B:301:3LS:OBK	0.80	2.40	2	2
2:B:301:3LS:OAA	2:B:301:3LS:SAK	0.78	2.42	3	2
2:B:301:3LS:SAK	2:B:301:3LS:CBI	0.66	2.83	4	4
2:B:301:3LS:SAK	2:B:301:3LS:CBH	0.65	2.85	4	1
2:B:301:3LS:SAK	2:B:301:3LS:OAU	0.64	2.56	4	1
1:C:261:THR:HG1	1:D:225:ARG:N	0.61	1.94	1	2
2:B:301:3LS:SAK	2:B:301:3LS:CBJ	0.60	2.89	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:260:THR:HG1	1:B:225:ARG:N	0.58	1.97	2	2
2:B:301:3LS:OBK	1:C:265:LYS:HE3	0.56	2.01	2	1
1:E:229:LYS:HB2	1:E:265:LYS:O	0.56	2.01	3	1
1:D:236:ARG:HD3	1:D:272:GLU:OE2	0.55	2.00	2	2
1:B:290:HIS:CD2	1:C:288:ASP:HB2	0.53	2.39	3	1
1:D:225:ARG:HD2	1:D:258:ASP:CG	0.52	2.24	1	1
1:A:230:ASP:O	1:A:266:THR:HA	0.52	2.04	4	1
1:E:233:THR:HB	1:E:237:ALA:HB3	0.51	1.82	4	1
1:C:274:ARG:HB3	1:C:287:TRP:CH2	0.50	2.41	3	2
1:C:281:TYR:HA	1:D:245:VAL:O	0.50	2.05	4	1
2:B:301:3LS:OAU	2:B:301:3LS:CBD	0.50	2.58	2	2
1:B:240:GLN:HB3	1:B:276:LEU:HD22	0.50	1.84	3	1
1:A:227:SER:O	1:A:263:SER:HA	0.50	2.07	1	1
1:E:225:ARG:O	1:E:261:THR:HA	0.49	2.07	3	2
1:D:269:GLY:HA2	1:E:233:THR:O	0.49	2.08	1	1
1:C:265:LYS:HB3	1:D:229:LYS:O	0.49	2.06	1	1
1:D:229:LYS:HB3	1:D:265:LYS:O	0.48	2.07	1	3
2:B:301:3LS:CAC	1:D:265:LYS:HE3	0.48	2.38	3	1
1:D:246:THR:OG1	1:D:282:GLY:HA3	0.48	2.09	1	3
1:D:225:ARG:HD3	1:D:258:ASP:OD2	0.47	2.08	3	1
1:A:282:GLY:O	1:B:246:THR:HA	0.47	2.10	2	2
1:D:227:SER:O	1:D:263:SER:HA	0.47	2.10	2	1
1:D:264:VAL:HA	1:E:228:ALA:O	0.47	2.09	2	1
1:E:229:LYS:HB3	1:E:265:LYS:O	0.47	2.10	2	1
1:B:264:VAL:HA	1:C:228:ALA:O	0.47	2.10	2	1
1:B:265:LYS:HB2	1:C:229:LYS:O	0.46	2.10	1	1
1:D:242:GLY:O	1:D:278:GLY:HA3	0.46	2.11	2	1
2:B:301:3LS:SAK	2:B:301:3LS:CBL	0.46	3.03	4	1
1:E:243:ASN:HB2	1:E:279:ASN:OD1	0.46	2.11	1	1
1:B:260:THR:OG1	1:C:225:ARG:HA	0.46	2.10	4	2
1:C:263:SER:O	1:D:227:SER:HA	0.45	2.11	3	1
1:C:276:LEU:HB2	1:C:287:TRP:CZ3	0.45	2.47	3	1
1:C:241:LEU:HD13	1:C:277:ILE:HB	0.44	1.87	3	1
1:B:229:LYS:HE3	2:B:301:3LS:OBG	0.44	2.13	2	1
1:A:246:THR:HG22	1:A:248:ALA:H	0.43	1.73	1	1
1:D:259:GLN:HE21	1:D:259:GLN:HA	0.43	1.71	4	1
1:E:283:GLY:HA2	1:E:290:HIS:CG	0.43	2.48	1	2
1:C:282:GLY:O	1:D:246:THR:HA	0.43	2.14	1	1
1:E:242:GLY:O	1:E:278:GLY:HA3	0.43	2.12	1	1
1:D:262:ASN:HA	1:E:226:ASN:O	0.43	2.14	3	1
1:D:287:TRP:CE3	1:D:288:ASP:HB3	0.43	2.49	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:286:PHE:CD2	1:C:244:VAL:HG11	0.43	2.48	1	1
1:C:229:LYS:HB3	1:C:265:LYS:O	0.42	2.14	1	1
1:E:246:THR:HG23	1:E:248:ALA:H	0.42	1.75	2	1
1:C:230:ASP:O	1:C:266:THR:HA	0.42	2.14	2	1
1:B:269:GLY:HA2	1:C:233:THR:O	0.42	2.15	4	1
1:D:265:LYS:HD2	1:D:265:LYS:N	0.41	2.30	3	1
2:B:301:3LS:OBK	1:C:229:LYS:HB2	0.41	2.16	1	1
1:C:232:ARG:HD3	1:C:234:GLU:OE2	0.41	2.16	1	1
1:E:227:SER:O	1:E:263:SER:HA	0.41	2.15	4	1
1:B:291:HIS:HA	1:C:289:ASN:OD1	0.40	2.16	1	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	69/79 (87%)	54±1 (79±2%)	13±1 (19±2%)	2±0 (2±1%)	10	49
1	B	69/79 (87%)	56±1 (82±2%)	12±1 (18±2%)	0±0 (1±1%)	26	73
1	C	69/79 (87%)	58±3 (84±4%)	10±3 (14±5%)	2±0 (2±1%)	10	49
1	D	69/79 (87%)	56±1 (82±1%)	12±1 (18±2%)	0±0 (0±1%)	38	78
1	E	69/79 (87%)	53±1 (77±2%)	14±1 (21±1%)	1±0 (2±1%)	12	54
All	All	1380/1580 (87%)	1111 (81%)	249 (18%)	20 (1%)	15	61

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	254	ILE	4
1	E	283	GLY	4
1	C	292	HIS	2
1	C	293	HIS	2
1	A	283	GLY	2
1	B	294	HIS	1
1	B	254	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	C	286	PHE	1
1	D	252	GLY	1
1	C	283	GLY	1
1	E	272	GLU	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	57/63 (90%)	50±1 (89±2%)	6±1 (11±2%)	9	52
1	B	57/63 (90%)	46±0 (82±1%)	10±0 (18±1%)	4	37
1	C	57/63 (90%)	47±1 (82±1%)	10±1 (18±1%)	4	39
1	D	57/63 (90%)	51±1 (89±2%)	6±1 (11±2%)	10	55
1	E	57/63 (90%)	46±2 (81±4%)	11±2 (19±4%)	4	36
All	All	1140/1260 (90%)	965 (85%)	175 (15%)	6	43

All 96 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	280	GLU	4
1	B	238	ARG	4
1	B	266	THR	4
1	B	276	LEU	4
1	B	280	GLU	4
1	C	233	THR	4
1	C	273	SER	4
1	C	276	LEU	4
1	E	238	ARG	4
1	E	255	ARG	4
1	E	276	LEU	4
1	E	287	TRP	4
1	A	266	THR	3
1	A	276	LEU	3
1	B	233	THR	3
1	C	258	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	C	261	THR	3
1	C	288	ASP	3
1	D	240	GLN	3
1	D	274	ARG	3
1	D	276	LEU	3
1	E	273	SER	3
1	E	288	ASP	3
1	B	292	HIS	3
1	E	274	ARG	3
1	E	280	GLU	3
1	A	233	THR	2
1	A	261	THR	2
1	A	265	LYS	2
1	B	251	HIS	2
1	C	259	GLN	2
1	C	279	ASN	2
1	D	238	ARG	2
1	D	286	PHE	2
1	C	230	ASP	2
1	C	281	TYR	2
1	C	291	HIS	2
1	E	270	LYS	2
1	B	263	SER	2
1	B	289	ASN	2
1	C	238	ARG	2
1	A	257	SER	1
1	A	292	HIS	1
1	B	235	GLU	1
1	B	250	LEU	1
1	B	257	SER	1
1	B	274	ARG	1
1	B	281	TYR	1
1	C	260	THR	1
1	D	255	ARG	1
1	D	266	THR	1
1	E	225	ARG	1
1	E	227	SER	1
1	E	229	LYS	1
1	E	234	GLU	1
1	E	258	ASP	1
1	E	272	GLU	1
1	E	279	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	E	284	LYS	1
1	A	227	SER	1
1	A	235	GLU	1
1	A	241	LEU	1
1	A	294	HIS	1
1	B	229	LYS	1
1	B	254	ILE	1
1	B	255	ARG	1
1	B	259	GLN	1
1	C	225	ARG	1
1	C	227	SER	1
1	D	225	ARG	1
1	D	230	ASP	1
1	D	246	THR	1
1	E	241	LEU	1
1	E	291	HIS	1
1	E	295	HIS	1
1	A	234	GLU	1
1	A	291	HIS	1
1	B	226	ASN	1
1	B	261	THR	1
1	B	265	LYS	1
1	C	266	THR	1
1	C	293	HIS	1
1	D	233	THR	1
1	D	281	TYR	1
1	A	255	ARG	1
1	A	273	SER	1
1	B	273	SER	1
1	B	291	HIS	1
1	C	257	SER	1
1	C	274	ARG	1
1	D	227	SER	1
1	D	259	GLN	1
1	D	263	SER	1
1	D	265	LYS	1
1	E	236	ARG	1
1	E	290	HIS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	3LS	B	301	-	23,43,43	1.41±0.02	2±0 (8±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	3LS	B	301	-	18,63,63	2.12±0.04	8±0 (44±0%)

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
2	3LS	B	301	-	-	0±0,12,32,32	0±0,5,5,5

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	301	3LS	CBD-CAO	2.78	1.33	1.37	2	4
2	B	301	3LS	CAY-CAG	2.62	1.33	1.37	3	4

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	301	3LS	CBH-CAZ-CAI	4.54	120.48	127.36	2	4
2	B	301	3LS	CBI-CBC-CAM	4.26	120.90	127.36	2	4
2	B	301	3LS	CBC-CAM-SAN	2.78	106.42	111.79	4	4
2	B	301	3LS	CAZ-CAI-SAH	2.48	106.99	111.79	4	4
2	B	301	3LS	OAV-CAC-CAD	2.38	120.10	114.69	1	4
2	B	301	3LS	OBG-CAS-CAR	2.30	119.93	114.69	4	4
2	B	301	3LS	OAA-CBJ-CBH	2.16	116.89	123.04	4	4
2	B	301	3LS	OAU-CBL-CBI	2.10	117.04	123.04	1	4

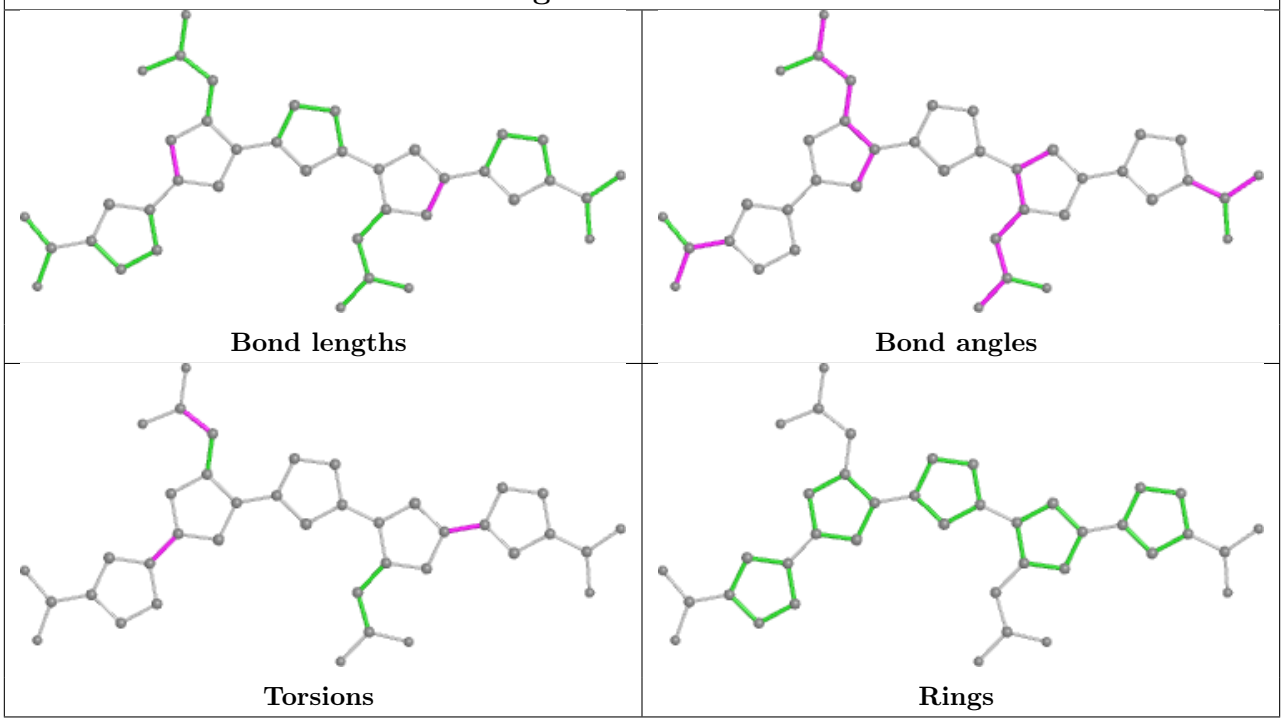
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 3LS B 301



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 6% for the well-defined parts and 6% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	320
Number of shifts mapped to atoms	304
Number of unparsed shifts	0
Number of shifts with mapping errors	16
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 16 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	222	ILE	C	175.1	0.2	1
1	A	222	ILE	CA	62.0	0.2	1
1	A	222	ILE	CB	38.3	0.2	1
1	A	222	ILE	CG1	27.5	0.2	1
1	A	222	ILE	CG2	18.7	0.2	1
1	A	222	ILE	CD1	13.0	0.2	1
1	A	222	ILE	N	128.9	0.2	9
1	A	223	VAL	C	175.95	0.2	9
1	A	223	VAL	CA	59.1	0.2	1
1	A	223	VAL	CB	32.4	0.2	1
1	A	223	VAL	CG1	22.2	0.2	9
1	A	223	VAL	CG2	19.7	0.2	9
1	A	223	VAL	N	125.4	0.2	1
1	A	224	GLY	C	178.5	0.2	9

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	224	GLY	CA	43.8	0.2	9
1	A	224	GLY	N	109.8	0.2	9

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	57	0.34 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	47	-0.73 ± 0.28	Should be checked
$^{13}C'$	56	0.64 ± 0.17	Should be applied
^{15}N	56	-1.80 ± 0.58	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 299 atoms were assigned a chemical shift out of a possible 4760. 0 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	160/1820 (9%)	0/755 (0%)	107/710 (15%)	53/355 (15%)
Sidechain	124/2540 (5%)	0/1635 (0%)	116/760 (15%)	8/145 (6%)
Aromatic	15/400 (4%)	0/215 (0%)	14/145 (10%)	1/40 (2%)
Overall	299/4760 (6%)	0/2605 (0%)	237/1615 (15%)	62/540 (11%)

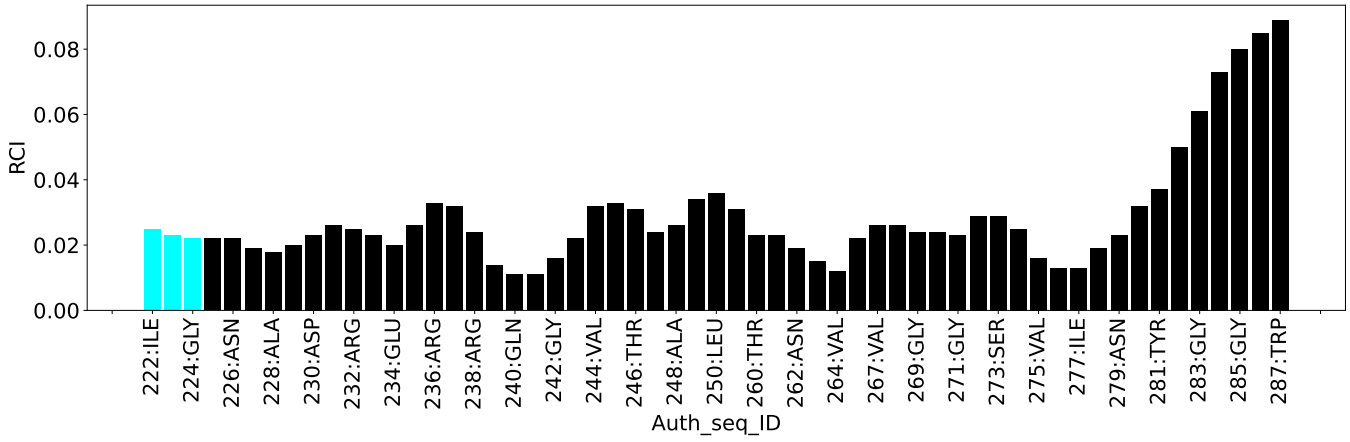
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 299 atoms were assigned a chemical shift out of a possible 4760. 0 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	160/1820 (9%)	0/755 (0%)	107/710 (15%)	53/355 (15%)
Sidechain	124/2540 (5%)	0/1635 (0%)	116/760 (15%)	8/145 (6%)
Aromatic	15/400 (4%)	0/215 (0%)	14/145 (10%)	1/40 (2%)
Overall	299/4760 (6%)	0/2605 (0%)	237/1615 (15%)	62/540 (11%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: