Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Aug 10, 2019 – 10:20 PM EDT

PDB ID	:	6GL7
EMDB ID:	:	EMD-0026
Title	:	Neurturin-GFRa2-RET extracellular complex
Authors	:	Bigalke, J.M.; Aibara, S.; Sandmark, J.; Amunts, A.
Deposited on	:	2018-05-23
Resolution	:	6.30 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

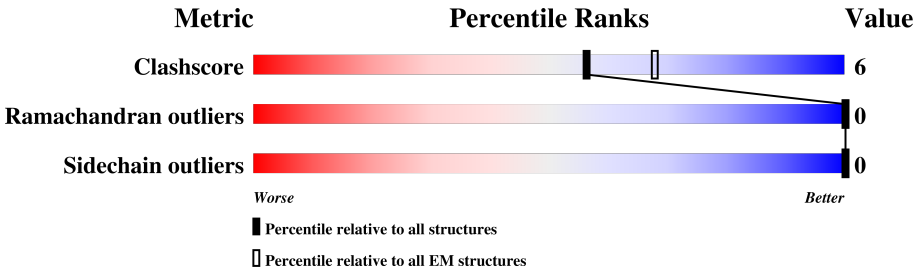
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	102	94%
1	B	102	93% 5%
2	C	426	66% 30%
2	D	426	64% 5% 30%
3	E	613	64% 9% 27%
3	F	613	65% 8% 27%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26510 atoms, of which 13004 are hydrogens and 0 are deuteriums.

In the tables below, 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 Neurturin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	100	Total	C	H	N	O	S	0	0
			1588	488	787	162	144	7		
1	A	100	Total	C	H	N	O	S	0	0
			1588	488	787	162	144	7		

- Molecule 2 is a protein called GDNF family receptor alpha-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	297	Total	C	H	N	O	S	0	0
			4582	1436	2233	431	449	33		
2	C	297	Total	C	H	N	O	S	0	0
			4582	1436	2233	431	449	33		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	442	HIS	-	expression tag	UNP O00451
D	443	HIS	-	expression tag	UNP O00451
D	444	HIS	-	expression tag	UNP O00451
D	445	HIS	-	expression tag	UNP O00451
D	446	HIS	-	expression tag	UNP O00451
D	447	HIS	-	expression tag	UNP O00451
C	442	HIS	-	expression tag	UNP O00451
C	443	HIS	-	expression tag	UNP O00451
C	444	HIS	-	expression tag	UNP O00451
C	445	HIS	-	expression tag	UNP O00451
C	446	HIS	-	expression tag	UNP O00451
C	447	HIS	-	expression tag	UNP O00451

- Molecule 3 is a protein called Proto-oncogene tyrosine-protein kinase receptor Ret.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	450	Total	C	H	N	O	S	0	0
			7085	2284	3482	637	667	15		
3	E	450	Total	C	H	N	O	S	0	0
			7085	2284	3482	637	667	15		

There are 12 discrepancies between the modelled and reference sequences:

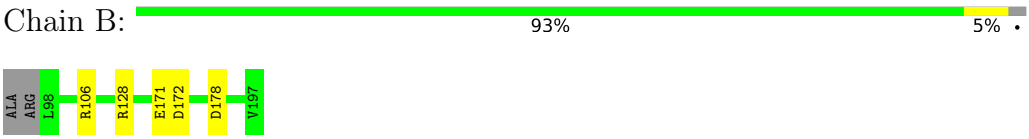
Chain	Residue	Modelled	Actual	Comment	Reference
F	636	GLU	-	expression tag	UNP P07949
F	637	ASN	-	expression tag	UNP P07949
F	638	LEU	-	expression tag	UNP P07949
F	639	TYR	-	expression tag	UNP P07949
F	640	PHE	-	expression tag	UNP P07949
F	641	GLN	-	expression tag	UNP P07949
E	636	GLU	-	expression tag	UNP P07949
E	637	ASN	-	expression tag	UNP P07949
E	638	LEU	-	expression tag	UNP P07949
E	639	TYR	-	expression tag	UNP P07949
E	640	PHE	-	expression tag	UNP P07949
E	641	GLN	-	expression tag	UNP P07949

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 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.

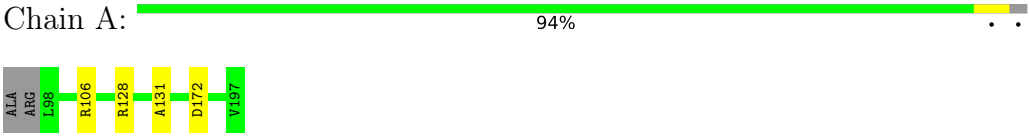
- Molecule 1: Neurturin

Chain B:



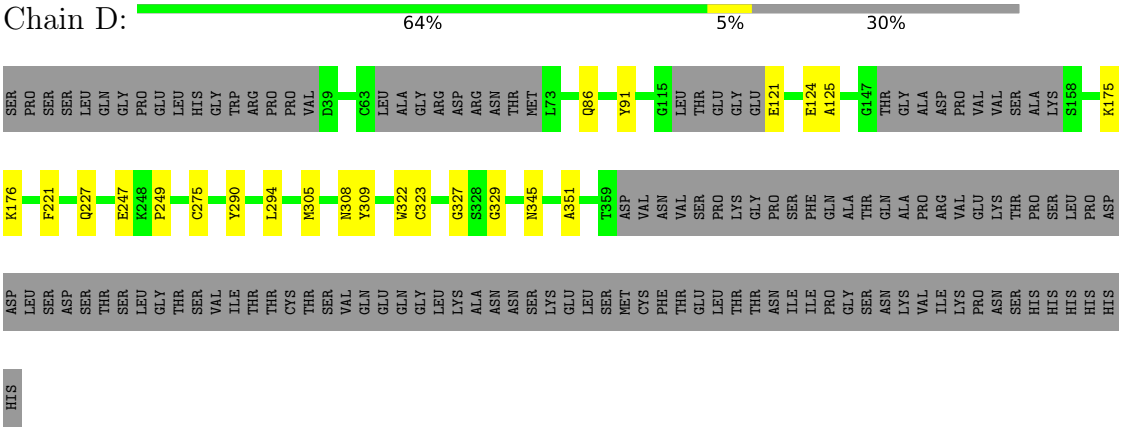
- Molecule 1: Neurturin

Chain A:



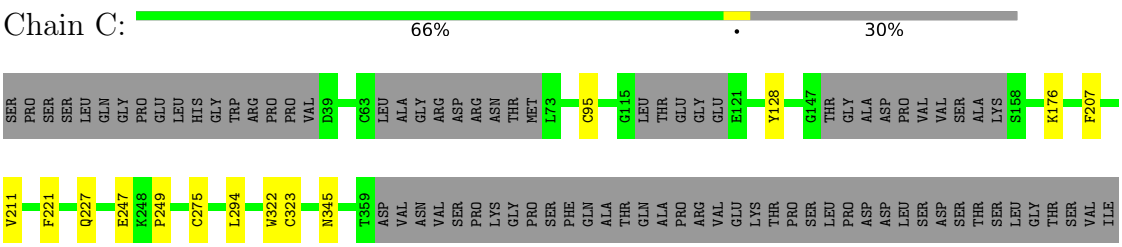
- Molecule 2: GDNF family receptor alpha-2

Chain D:



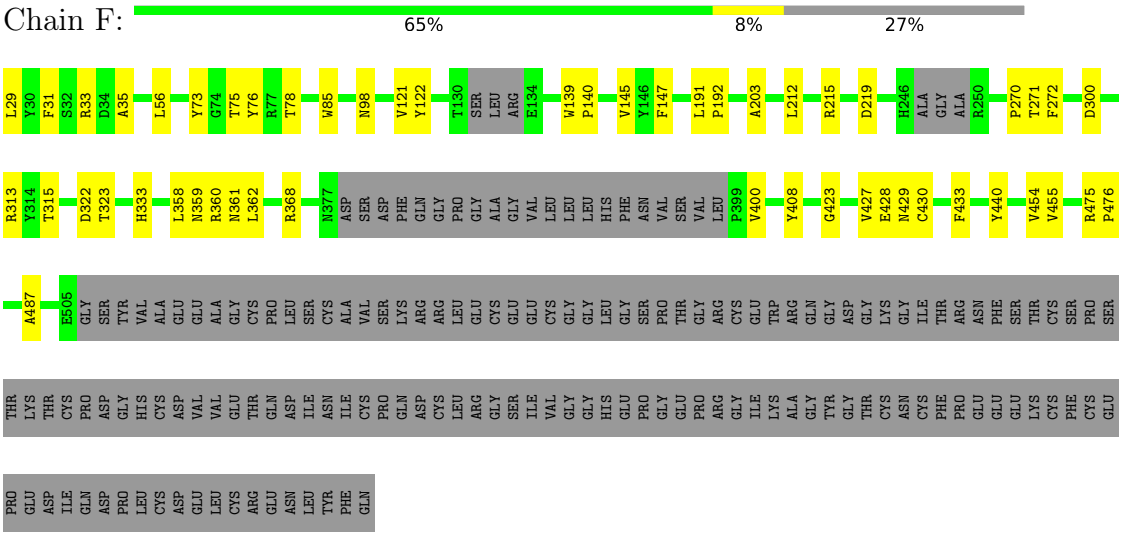
- Molecule 2: GDNF family receptor alpha-2

Chain C:



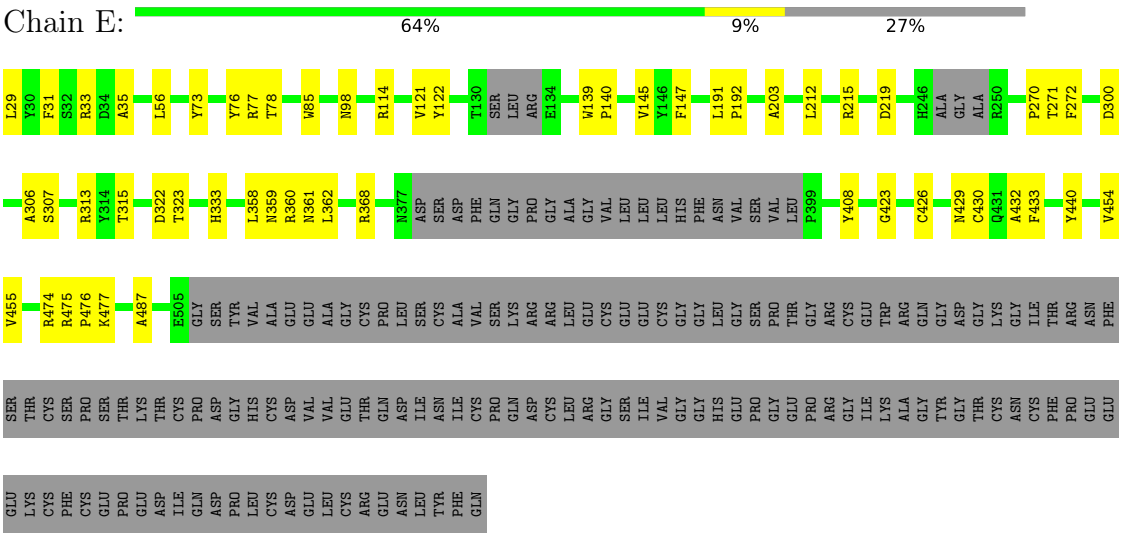
• Molecule 3: Proto-oncogene tyrosine-protein kinase receptor Ret

Chain F:



• Molecule 3: Proto-oncogene tyrosine-protein kinase receptor Ret

Chain E:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	186903	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.77	0/813	0.56	0/1092
1	B	0.78	0/813	0.54	0/1092
2	C	0.65	0/2390	0.49	0/3216
2	D	0.67	0/2390	0.49	0/3216
3	E	0.65	0/3690	0.56	0/5022
3	F	0.65	0/3690	0.56	0/5022
All	All	0.67	0/13786	0.54	0/18660

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

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	801	787	786	3	0
1	B	801	787	786	4	0
2	C	2349	2233	2229	8	0
2	D	2349	2233	2229	26	0
3	E	3603	3482	3527	68	0
3	F	3603	3482	3527	57	0
All	All	13506	13004	13084	148	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 6.

All (148) 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:E:271:THR:CG2	3:E:300:ASP:HB3	1.64	1.25
3:E:271:THR:CG2	3:E:300:ASP:CB	2.18	1.22
3:F:271:THR:HG22	3:F:300:ASP:CB	1.70	1.20
3:F:271:THR:HG22	3:F:300:ASP:HB3	1.29	1.08
2:D:121:GLU:HG3	3:E:77:ARG:NH1	1.71	1.06
2:D:329:GLY:HA3	3:E:306:ALA:HB2	1.31	1.05
3:E:271:THR:HG21	3:E:300:ASP:HB3	1.37	1.05
3:E:271:THR:HG22	3:E:300:ASP:CB	1.80	1.05
3:E:271:THR:HG22	3:E:300:ASP:HB3	1.35	1.01
3:E:271:THR:CG2	3:E:300:ASP:HB2	1.95	0.97
3:F:271:THR:HG22	3:F:300:ASP:HB2	1.46	0.95
3:F:271:THR:OG1	3:F:368:ARG:HG3	1.69	0.93
3:F:271:THR:CG2	3:F:300:ASP:CB	2.48	0.92
3:E:271:THR:HB	3:E:272:PHE:CG	2.10	0.87
3:F:271:THR:CG2	3:F:300:ASP:HB3	2.06	0.86
3:F:271:THR:CG2	3:F:300:ASP:HB2	2.05	0.85
3:F:333:HIS:CE1	3:F:358:LEU:HD22	2.13	0.84
3:E:333:HIS:CE1	3:E:358:LEU:HD22	2.14	0.82
3:E:271:THR:HB	3:E:272:PHE:CD1	2.17	0.79
2:D:329:GLY:HA3	3:E:306:ALA:CB	2.13	0.79
3:F:333:HIS:CE1	3:F:358:LEU:CD2	2.66	0.79
3:E:333:HIS:CE1	3:E:358:LEU:CD2	2.67	0.77
2:D:121:GLU:HG3	3:E:77:ARG:CZ	2.17	0.73
3:F:333:HIS:ND1	3:F:358:LEU:CD2	2.52	0.73
3:E:333:HIS:ND1	3:E:358:LEU:CD2	2.52	0.72
3:F:427:VAL:HG23	3:F:429:ASN:HB2	1.72	0.72
3:E:271:THR:HG21	3:E:300:ASP:CB	2.07	0.70
3:E:271:THR:HG23	3:E:300:ASP:HB2	1.72	0.70
3:F:427:VAL:CG2	3:F:429:ASN:HB2	2.22	0.69
3:F:31:PHE:HB2	3:F:139:TRP:CD1	2.27	0.69
2:D:327:GLY:O	3:E:307:SER:N	2.22	0.69
2:D:91:TYR:OH	3:E:114:ARG:HD3	1.93	0.68
3:E:333:HIS:ND1	3:E:358:LEU:HD23	2.09	0.68
3:F:333:HIS:ND1	3:F:358:LEU:HD23	2.08	0.67
3:E:271:THR:OG1	3:E:368:ARG:HG3	2.00	0.62
3:F:360:ARG:HE	3:F:361:ASN:ND2	1.97	0.62
3:E:360:ARG:HE	3:E:361:ASN:ND2	1.97	0.61
3:F:428:GLU:OE1	3:F:428:GLU:N	2.31	0.61
3:E:315:THR:HG21	3:E:362:LEU:HB2	1.82	0.61
3:F:333:HIS:ND1	3:F:358:LEU:HD22	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:270:PRO:O	3:E:271:THR:CG2	2.50	0.60
3:F:315:THR:HG21	3:F:362:LEU:HB2	1.83	0.60
2:D:121:GLU:N	3:E:77:ARG:NH2	2.50	0.59
3:E:333:HIS:ND1	3:E:358:LEU:HD22	2.17	0.59
3:F:31:PHE:HB2	3:F:139:TRP:NE1	2.18	0.58
3:F:139:TRP:CG	3:F:140:PRO:HA	2.40	0.56
3:F:430:CYS:HA	3:F:433:PHE:CZ	2.40	0.56
3:E:139:TRP:CG	3:E:140:PRO:HA	2.40	0.56
3:E:315:THR:HG21	3:E:362:LEU:CB	2.35	0.56
3:F:315:THR:HG21	3:F:362:LEU:CB	2.36	0.56
3:E:271:THR:HG22	3:E:300:ASP:CA	2.35	0.55
3:E:270:PRO:O	3:E:271:THR:HG23	2.07	0.55
3:F:333:HIS:CE1	3:F:358:LEU:HD23	2.42	0.55
3:E:359:ASN:OD1	3:E:360:ARG:N	2.40	0.55
2:D:124:GLU:O	3:E:76:TYR:CE1	2.60	0.54
3:F:359:ASN:OD1	3:F:360:ARG:N	2.40	0.54
3:E:315:THR:HG21	3:E:362:LEU:N	2.24	0.53
3:F:315:THR:HG21	3:F:362:LEU:N	2.25	0.52
3:F:271:THR:HB	3:F:272:PHE:CG	2.45	0.52
3:F:270:PRO:C	3:F:271:THR:HG23	2.30	0.51
3:E:322:ASP:OD1	3:E:323:THR:N	2.43	0.51
3:E:333:HIS:CE1	3:E:358:LEU:HD23	2.42	0.51
2:D:121:GLU:N	3:E:77:ARG:CZ	2.74	0.51
3:F:322:ASP:OD1	3:F:323:THR:N	2.43	0.51
1:B:172:ASP:OD2	2:D:176:LYS:NZ	2.45	0.50
1:B:171:GLU:OE1	2:D:175:LYS:NZ	2.42	0.50
1:A:106:ARG:NH1	1:A:131:ALA:O	2.45	0.50
2:C:275:CYS:O	2:C:345:ASN:ND2	2.45	0.50
3:E:430:CYS:HA	3:E:433:PHE:CZ	2.47	0.49
3:F:31:PHE:HB2	3:F:139:TRP:HE1	1.76	0.49
2:D:121:GLU:HG3	3:E:77:ARG:HH12	1.72	0.49
3:F:122:TYR:HA	3:F:145:VAL:O	2.13	0.49
3:F:271:THR:HB	3:F:272:PHE:CD1	2.48	0.48
3:F:360:ARG:HE	3:F:361:ASN:HD22	1.60	0.48
3:F:139:TRP:CD2	3:F:140:PRO:HA	2.47	0.48
3:E:139:TRP:CD1	3:E:140:PRO:HA	2.48	0.48
2:D:125:ALA:HA	3:E:76:TYR:CZ	2.48	0.48
2:D:275:CYS:O	2:D:345:ASN:ND2	2.46	0.48
3:E:122:TYR:HA	3:E:145:VAL:O	2.13	0.48
2:D:327:GLY:O	3:E:307:SER:CB	2.62	0.48
3:E:271:THR:HB	3:E:272:PHE:CD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:270:PRO:C	3:E:271:THR:HG23	2.35	0.47
3:E:31:PHE:HB2	3:E:139:TRP:CD1	2.49	0.47
3:E:360:ARG:HE	3:E:361:ASN:HD22	1.60	0.47
3:F:400:VAL:HB	3:F:429:ASN:OD1	2.14	0.47
3:E:440:TYR:HA	3:E:487:ALA:HB2	1.96	0.47
3:F:313:ARG:HD3	3:F:361:ASN:OD1	2.14	0.47
3:E:313:ARG:HD3	3:E:361:ASN:OD1	2.14	0.47
3:F:440:TYR:HA	3:F:487:ALA:HB2	1.96	0.46
3:E:212:LEU:O	3:E:215:ARG:NH1	2.48	0.46
3:E:454:VAL:O	3:E:454:VAL:HG12	2.15	0.46
3:F:454:VAL:HG12	3:F:454:VAL:O	2.15	0.46
3:F:427:VAL:HG21	3:F:440:TYR:OH	2.16	0.46
2:D:221:PHE:CE2	2:D:294:LEU:HB3	2.50	0.46
2:D:305:MET:HG3	2:D:305:MET:O	2.15	0.46
3:F:212:LEU:O	3:F:215:ARG:NH1	2.48	0.46
3:E:455:VAL:HG23	3:E:455:VAL:O	2.15	0.45
3:F:455:VAL:HG23	3:F:455:VAL:O	2.15	0.45
3:F:429:ASN:O	3:F:433:PHE:CD2	2.69	0.45
3:F:73:TYR:HA	3:F:78:THR:O	2.16	0.45
3:E:121:VAL:O	3:E:147:PHE:N	2.49	0.45
3:F:427:VAL:HG21	3:F:429:ASN:HB2	1.97	0.44
1:B:106:ARG:O	1:B:128:ARG:HA	2.18	0.44
3:F:121:VAL:O	3:F:147:PHE:N	2.49	0.44
2:D:247:GLU:O	2:D:322:TRP:NE1	2.51	0.44
2:D:249:PRO:O	2:D:323:CYS:HB2	2.17	0.44
2:D:121:GLU:CG	3:E:77:ARG:NH1	2.62	0.44
3:E:73:TYR:HA	3:E:78:THR:O	2.16	0.44
3:E:85:TRP:O	3:E:98:ASN:N	2.52	0.43
1:A:106:ARG:O	1:A:128:ARG:HA	2.18	0.43
3:E:475:ARG:N	3:E:476:PRO:HD2	2.33	0.43
3:F:475:ARG:N	3:F:476:PRO:HD2	2.33	0.43
2:C:95:CYS:HB3	2:C:128:TYR:HA	1.99	0.43
2:D:290:TYR:CD1	2:D:351:ALA:HA	2.54	0.43
3:F:408:TYR:CZ	3:F:423:GLY:HA3	2.54	0.43
1:A:172:ASP:OD2	2:C:176:LYS:NZ	2.52	0.43
2:C:227:GLN:N	2:C:227:GLN:OE1	2.52	0.43
2:D:308:ASN:OD1	2:D:309:TYR:N	2.51	0.43
3:E:408:TYR:CZ	3:E:423:GLY:HA3	2.54	0.43
3:F:85:TRP:O	3:F:98:ASN:N	2.52	0.43
2:D:125:ALA:HA	3:E:76:TYR:CE2	2.54	0.43
3:E:33:ARG:HD3	3:E:35:ALA:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:33:ARG:HD3	3:F:35:ALA:O	2.19	0.42
3:E:29:LEU:HA	3:E:56:LEU:O	2.19	0.42
2:C:249:PRO:O	2:C:323:CYS:HB2	2.20	0.42
3:E:191:LEU:N	3:E:192:PRO:HD2	2.35	0.42
3:E:203:ALA:HB1	3:E:219:ASP:HA	2.02	0.42
3:E:426:CYS:SG	3:E:430:CYS:SG	3.13	0.42
3:F:191:LEU:N	3:F:192:PRO:HD2	2.35	0.42
3:F:29:LEU:HA	3:F:56:LEU:O	2.19	0.42
2:D:227:GLN:N	2:D:227:GLN:OE1	2.52	0.41
2:C:247:GLU:O	2:C:322:TRP:NE1	2.53	0.41
2:C:221:PHE:CE2	2:C:294:LEU:HD11	2.55	0.41
3:F:203:ALA:HB1	3:F:219:ASP:HA	2.02	0.41
2:D:327:GLY:O	3:E:307:SER:HB3	2.20	0.41
2:D:86:GLN:HA	2:D:91:TYR:CG	2.56	0.41
3:F:270:PRO:C	3:F:271:THR:CG2	2.88	0.41
3:F:427:VAL:O	3:F:430:CYS:SG	2.79	0.41
3:F:75:THR:HG22	3:F:76:TYR:CD2	2.56	0.41
3:E:333:HIS:CE1	3:E:358:LEU:HB3	2.56	0.41
3:F:333:HIS:CE1	3:F:358:LEU:HA	2.56	0.41
2:C:207:PHE:CE1	2:C:211:VAL:HG21	2.56	0.40
3:E:474:ARG:CZ	3:E:477:LYS:HG2	2.51	0.40
3:E:429:ASN:HA	3:E:432:ALA:HB3	2.03	0.40
3:F:333:HIS:CE1	3:F:358:LEU:HB3	2.56	0.40
3:E:333:HIS:CE1	3:E:358:LEU:HA	2.57	0.40
3:F:271:THR:HB	3:F:272:PHE:CD2	2.57	0.40
1:B:178:ASP:OD1	1:B:178:ASP:C	2.59	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 PDB entries followed by that with respect to all EM 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	98/102 (96%)	97 (99%)	1 (1%)	0	100	100
1	B	98/102 (96%)	97 (99%)	1 (1%)	0	100	100
2	C	289/426 (68%)	280 (97%)	9 (3%)	0	100	100
2	D	289/426 (68%)	277 (96%)	12 (4%)	0	100	100
3	E	442/613 (72%)	418 (95%)	24 (5%)	0	100	100
3	F	442/613 (72%)	418 (95%)	24 (5%)	0	100	100
All	All	1658/2282 (73%)	1587 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM 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	82/83 (99%)	82 (100%)	0	100	100
1	B	82/83 (99%)	82 (100%)	0	100	100
2	C	263/377 (70%)	263 (100%)	0	100	100
2	D	263/377 (70%)	263 (100%)	0	100	100
3	E	399/534 (75%)	399 (100%)	0	100	100
3	F	399/534 (75%)	399 (100%)	0	100	100
All	All	1488/1988 (75%)	1488 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.