Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2024 – 07:08 PM JST

PDB ID	:	8J9B
Title	:	LnaB-actin binary complex
Deposited on	:	2023-05-03
Resolution	:	3.42 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

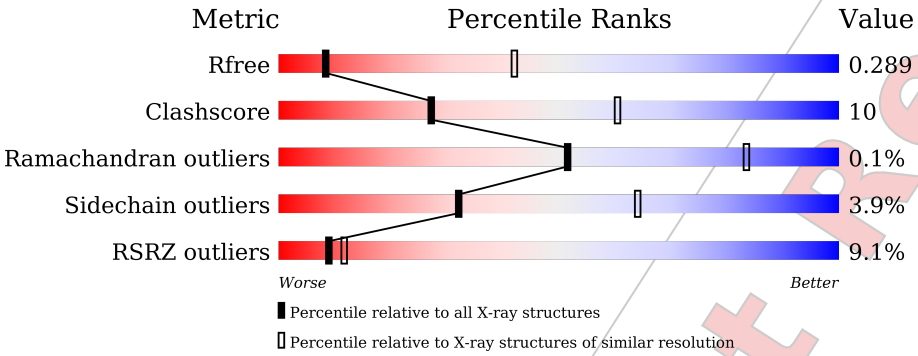
For Manuscript Review

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 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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% 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	375	21% 62% 22% • 14%
1	B	375	14% 65% 26% • 9%
1	C	375	5% 70% 20% • 9%
1	D	375	5% 71% 22% • 6%
1	E	375	8% 65% 19% • 15%
1	F	375	6% 70% 19% • 10%

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	441	4% 64% 14% 21%
2	I	441	6% 59% 16% 24%
2	J	441	3% 63% 15% 22%
2	K	441	7% 61% 14% 25%

For Manuscript Review

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26804 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 Actin gamma 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2538	1619	420	479	20			
1	B	343	Total	C	N	O	S	0	0	0
			2683	1706	446	511	20			
1	C	342	Total	C	N	O	S	0	0	0
			2673	1700	439	514	20			
1	D	354	Total	C	N	O	S	0	0	0
			2774	1763	462	529	20			
1	E	318	Total	C	N	O	S	0	0	0
			2488	1585	410	474	19			
1	F	338	Total	C	N	O	S	0	0	0
			2641	1676	443	502	20			

- Molecule 2 is a protein called Type IV secretion protein Dot.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	348	Total	C	N	O	S	0	0	0
			2826	1803	462	556	5			
2	I	335	Total	C	N	O	S	0	0	0
			2707	1723	444	535	5			
2	J	343	Total	C	N	O	S	0	0	0
			2780	1772	457	546	5			
2	K	331	Total	C	N	O	S	0	0	0
			2694	1726	442	521	5			

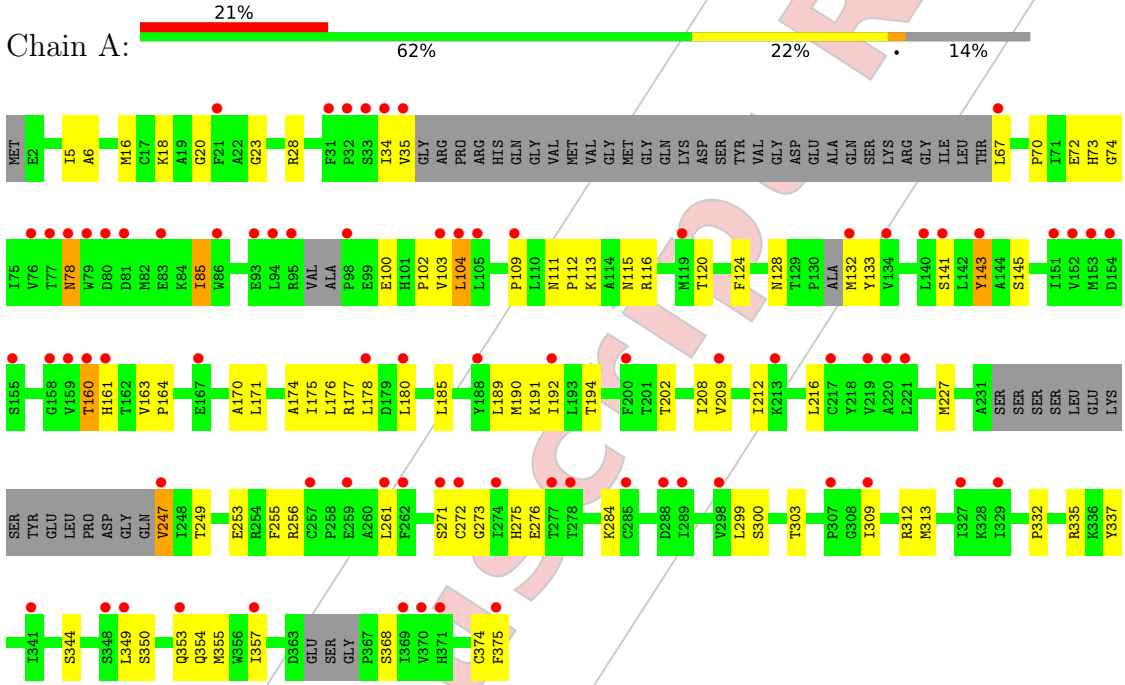
For Manuscript Review

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 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.

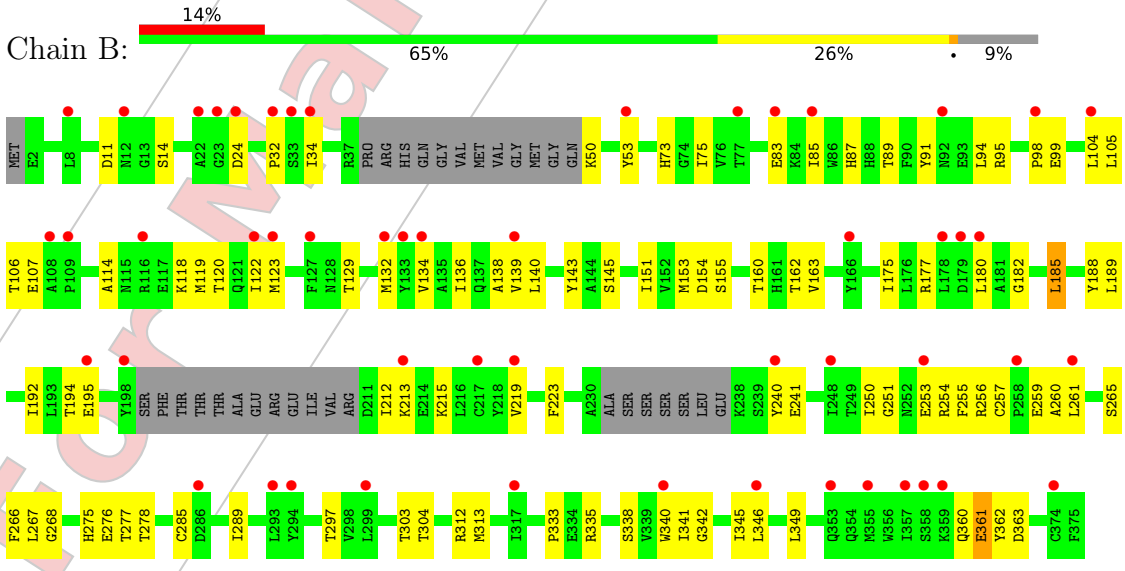
• Molecule 1: Actin gamma 1

Chain A:



• Molecule 1: Actin gamma 1

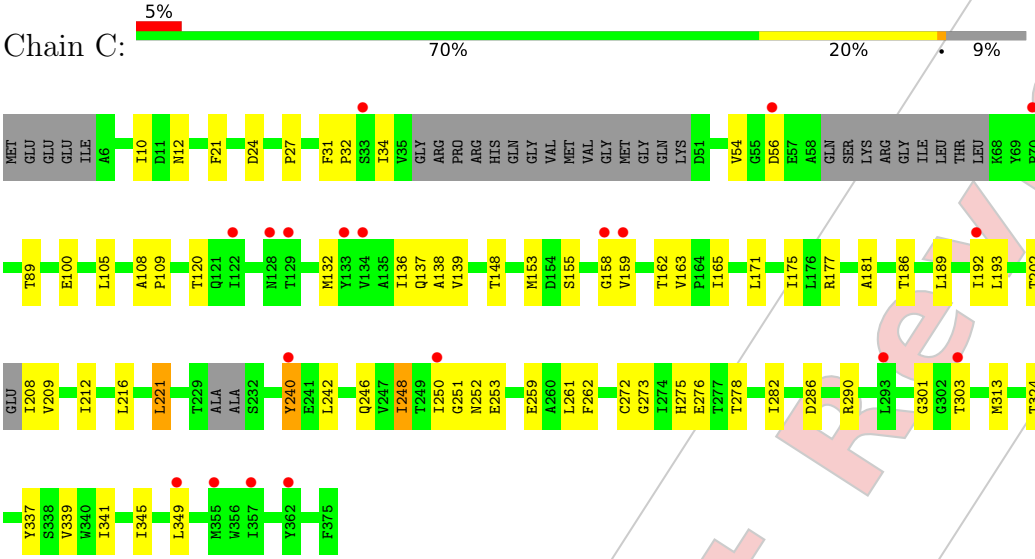
Chain B:



For Manuscript Review

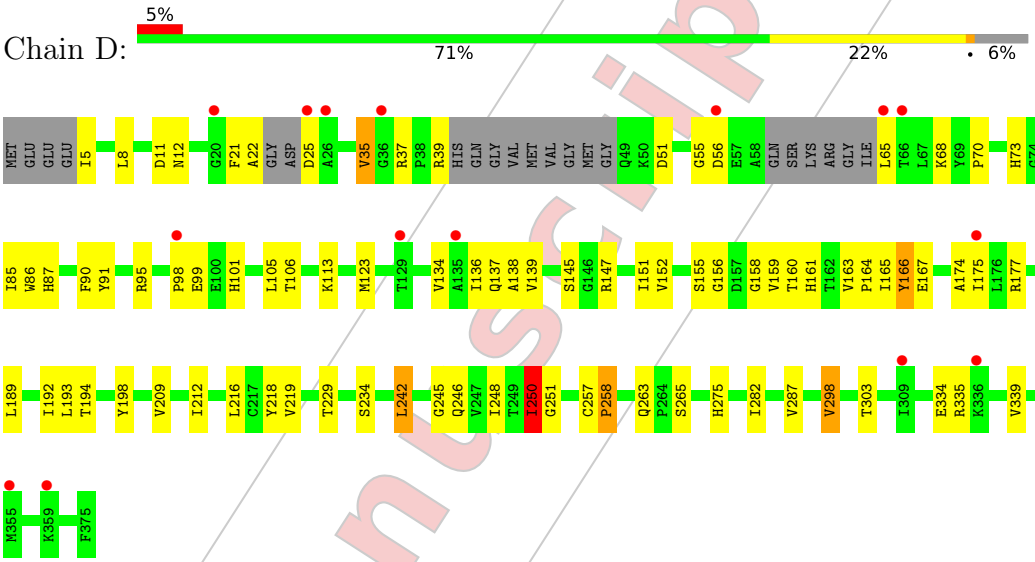
• Molecule 1: Actin gamma 1

Chain C:



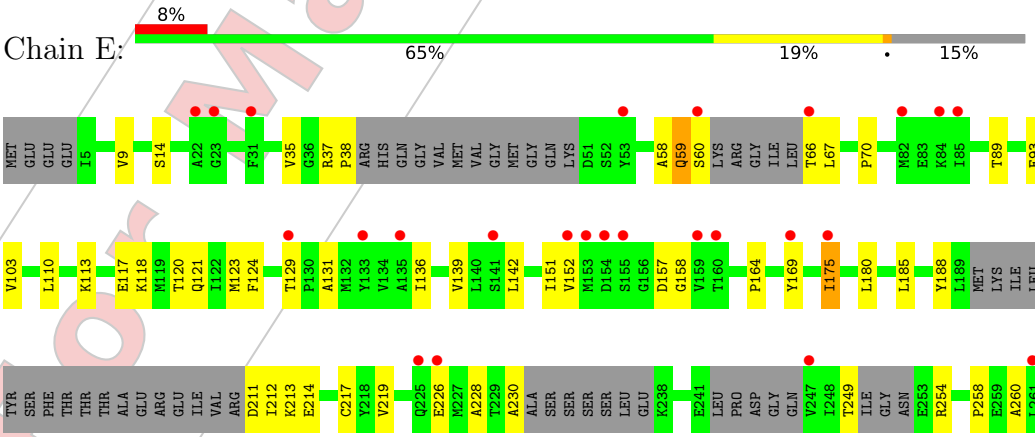
• Molecule 1: Actin gamma 1

Chain D:

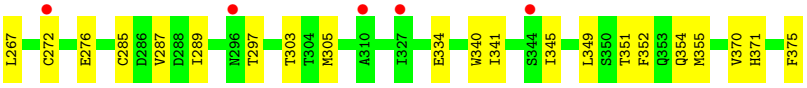


• Molecule 1: Actin gamma 1

Chain E:



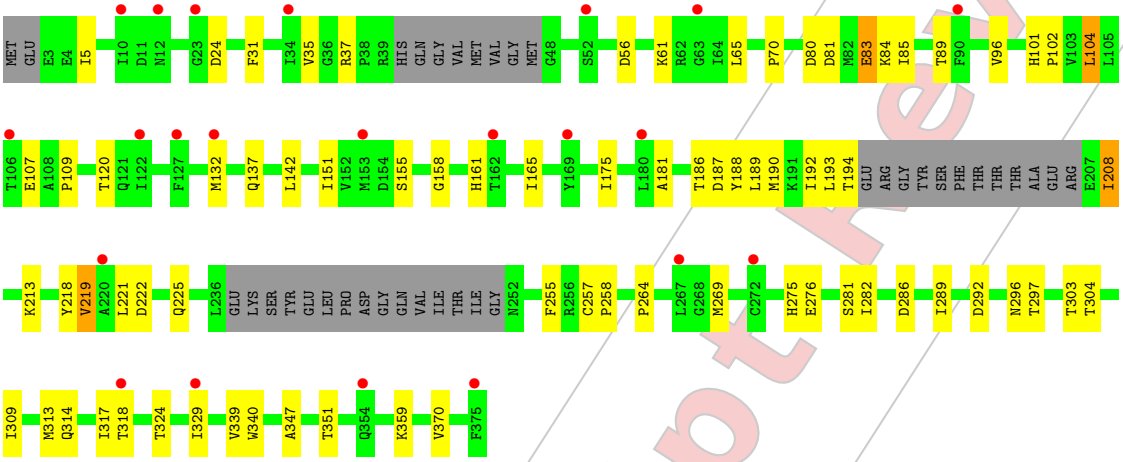
For Manuscript Review



• Molecule 1: Actin gamma 1

Chain F:

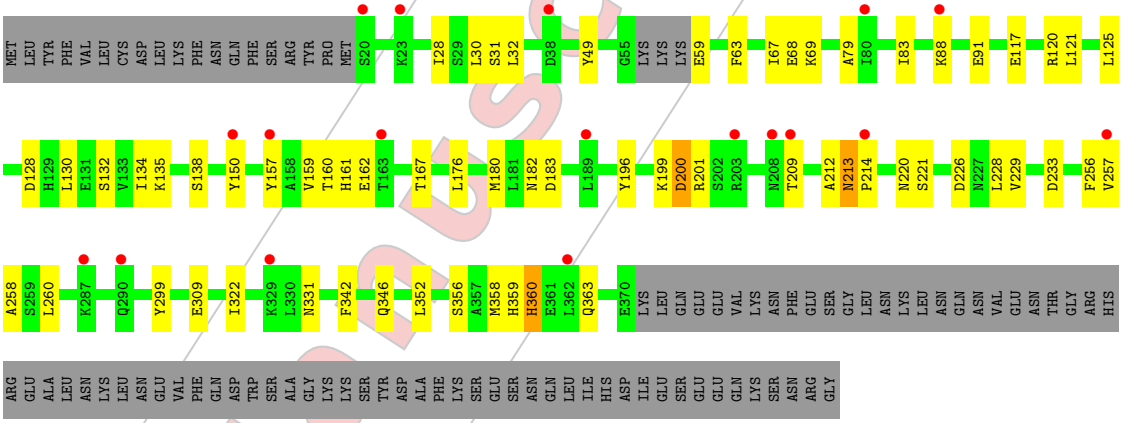




• Molecule 2: Type IV secretion protein Dot

Chain H:

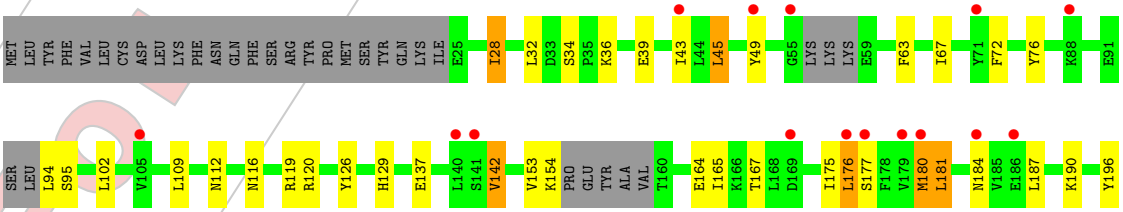




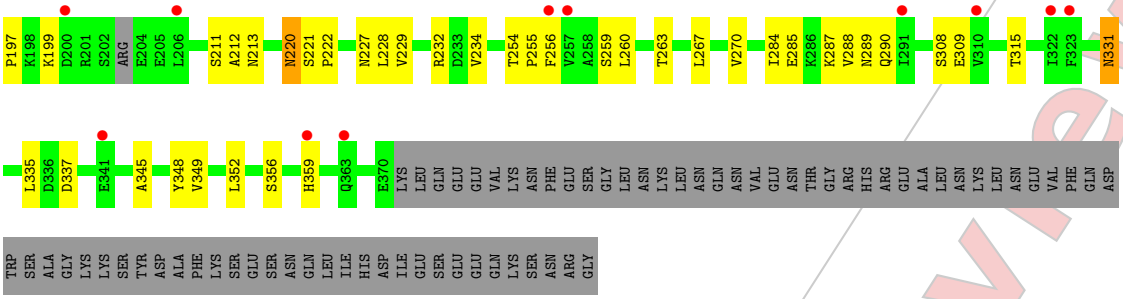
• Molecule 2: Type IV secretion protein Dot

Chain I:





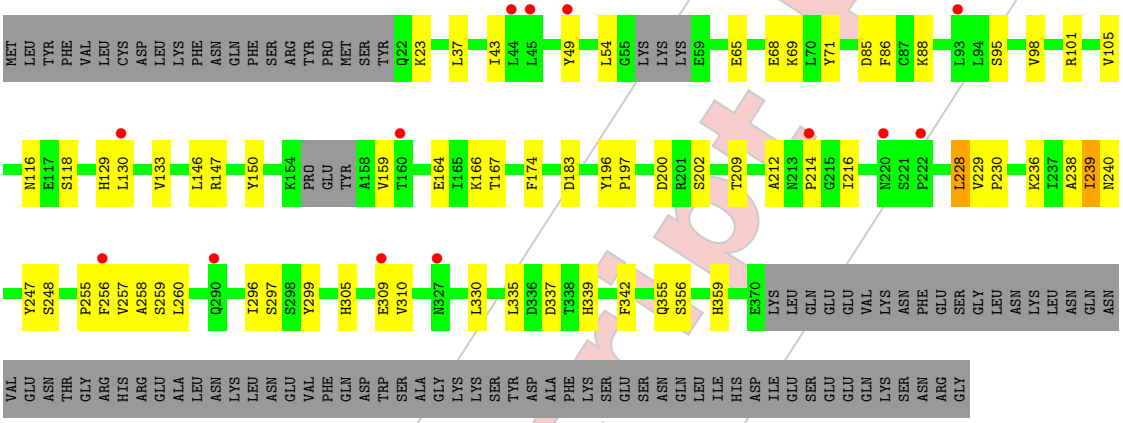
For Manuscript Review



• Molecule 2: Type IV secretion protein Dot

Chain J:

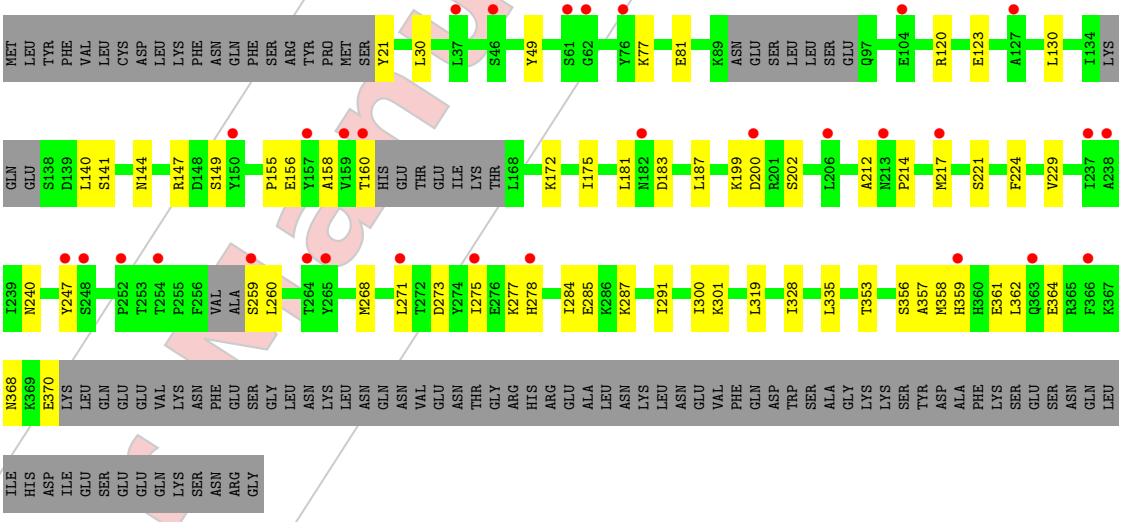




• Molecule 2: Type IV secretion protein Dot

Chain K:





For Manuscript Review

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	110.58Å 110.58Å 407.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.10 – 3.42 135.98 – 3.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.10-3.42) 99.9 (135.98-3.42)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.287 , 0.298 0.289 , 0.289	Depositor DCC
R_{free} test set	3809 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	73.3	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.018 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	26804	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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.

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

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	0.81	0/2591	0.89	2/3502 (0.1%)
1	B	0.87	0/2740	0.88	0/3706
1	C	1.03	0/2730	0.93	5/3697 (0.1%)
1	D	1.03	0/2833	0.92	6/3835 (0.2%)
1	E	0.99	0/2541	0.88	3/3438 (0.1%)
1	F	1.00	0/2696	0.89	0/3646
2	H	1.04	0/2881	0.90	3/3889 (0.1%)
2	I	1.01	0/2755	0.93	5/3713 (0.1%)
2	J	0.85	0/2831	0.85	4/3818 (0.1%)
2	K	0.72	0/2745	0.72	2/3698 (0.1%)
All	All	0.94	0/27343	0.88	30/36942 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	187	LEU	CA-CB-CG	5.99	129.08	115.30
2	I	137	GLU	N-CA-C	-5.95	94.95	111.00
2	J	228	LEU	N-CA-C	-5.95	94.94	111.00
1	D	98	PRO	N-CA-C	5.82	127.23	112.10
2	H	138	SER	N-CA-C	5.81	126.68	111.00
1	D	242	LEU	CA-CB-CG	5.75	128.52	115.30
2	J	240	ASN	N-CA-C	-5.74	95.51	111.00
1	E	272	CYS	N-CA-C	5.72	126.45	111.00
1	D	250	ILE	CB-CA-C	-5.70	100.20	111.60
1	C	100	GLU	N-CA-CB	-5.70	100.34	110.60
1	E	157	ASP	N-CA-C	-5.69	95.65	111.00
1	A	247	VAL	N-CA-CB	5.68	124.00	111.50
2	I	267	LEU	N-CA-C	-5.65	95.75	111.00
2	H	352	LEU	CA-CB-CG	5.60	128.18	115.30
2	I	164	GLU	N-CA-C	-5.56	95.99	111.00
1	D	35	VAL	N-CA-C	-5.55	96.02	111.00
2	J	37	LEU	CA-CB-CG	5.48	127.91	115.30

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	375	PHE	CB-CA-C	-5.45	99.51	110.40
1	C	163	VAL	CB-CA-C	-5.43	101.07	111.40
2	K	181	LEU	N-CA-C	-5.39	96.43	111.00
2	I	352	LEU	CA-CB-CG	5.34	127.58	115.30
1	D	55	GLY	N-CA-C	5.33	126.44	113.10
1	C	272	CYS	N-CA-C	5.31	125.34	111.00
2	J	239	ILE	CB-CA-C	-5.30	101.00	111.60
2	H	331	ASN	N-CA-C	-5.20	96.96	111.00
1	D	251	GLY	N-CA-C	-5.17	100.17	113.10
1	C	221	LEU	N-CA-C	-5.13	97.14	111.00
1	C	349	LEU	CA-CB-CG	5.13	127.10	115.30
2	I	142	VAL	N-CA-C	-5.10	97.24	111.00
1	A	249	THR	N-CA-C	-5.08	97.27	111.00

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	2538	0	2511	62	0
1	B	2683	0	2645	100	0
1	C	2673	0	2626	48	0
1	D	2774	0	2746	60	0
1	E	2488	0	2443	49	0
1	F	2641	0	2618	52	0
2	H	2826	0	2816	34	0
2	I	2707	0	2686	56	0
2	J	2780	0	2779	47	0
2	K	2694	0	2696	36	0
All	All	26804	0	26566	540	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 10.

All (540) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

For Manuscript Review

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:157:TYR:CD2	2:H:180:MET:HE3	1.51	1.45
1:B:105:LEU:HD21	1:B:123:MET:CE	1.69	1.21
1:B:143:TYR:CD2	1:B:346:LEU:HD11	1.77	1.19
2:H:157:TYR:CD2	2:H:180:MET:CE	2.26	1.18
2:H:157:TYR:HD2	2:H:180:MET:CE	1.57	1.17
2:I:176:LEU:HD23	2:I:177:SER:N	1.57	1.17
1:A:208:ILE:CG2	1:A:247:VAL:HG21	1.79	1.13
1:C:202:THR:HG22	1:C:203:THR:H	1.07	1.12
1:A:34:ILE:HG21	1:A:67:LEU:HD22	1.31	1.12
1:F:35:VAL:HG12	1:F:37:ARG:NH2	1.67	1.06
1:B:192:ILE:HD12	1:B:253:GLU:HG2	1.30	1.06
1:F:35:VAL:HG12	1:F:37:ARG:HH21	0.93	1.06
1:A:208:ILE:HG23	1:A:247:VAL:CG2	1.85	1.04
1:B:192:ILE:HD12	1:B:253:GLU:CG	1.87	1.04
1:C:202:THR:HG22	1:C:203:THR:N	1.73	1.02
1:E:212:ILE:HG23	1:E:212:ILE:O	1.61	1.01
1:F:35:VAL:CG1	1:F:37:ARG:HH21	1.74	0.99
1:F:35:VAL:CG1	1:F:37:ARG:NH2	2.25	0.98
1:A:208:ILE:HG23	1:A:247:VAL:HG21	1.40	0.98
1:B:105:LEU:CD2	1:B:123:MET:HE1	1.92	0.98
1:B:143:TYR:CE2	1:B:346:LEU:HD11	1.98	0.98
1:B:192:ILE:HD12	1:B:253:GLU:HB3	1.44	0.97
1:B:192:ILE:HD12	1:B:253:GLU:CB	1.94	0.95
1:C:202:THR:CG2	1:C:203:THR:H	1.80	0.94
1:B:105:LEU:HD21	1:B:123:MET:HE1	0.95	0.94
1:C:155:SER:HB3	1:C:303:THR:HB	1.50	0.93
2:I:176:LEU:HD23	2:I:177:SER:CA	2.01	0.91
1:B:155:SER:OG	1:B:304:THR:HG23	1.70	0.90
1:B:192:ILE:CD1	1:B:253:GLU:HB3	2.03	0.88
1:B:143:TYR:HD2	1:B:346:LEU:HD11	1.38	0.87
1:B:189:LEU:HD12	1:B:192:ILE:HD11	1.56	0.87
2:J:355:GLN:O	2:J:359:HIS:CG	2.27	0.87
1:A:208:ILE:CG2	1:A:247:VAL:CG2	2.50	0.86
1:C:186:THR:HG23	1:C:209:VAL:HG23	1.56	0.86
1:A:34:ILE:HG21	1:A:67:LEU:CD2	2.07	0.85
1:B:250:ILE:HG22	1:B:254:ARG:CG	2.09	0.83
1:B:188:TYR:CZ	1:B:266:PHE:HB3	2.14	0.83
2:I:176:LEU:CD2	2:I:177:SER:N	2.40	0.83
1:B:120:THR:HG22	1:B:362:TYR:CE2	2.14	0.82
1:A:34:ILE:CG2	1:A:67:LEU:HD22	2.10	0.81
1:D:5:ILE:CG2	1:D:101:HIS:ND1	2.44	0.81
1:B:119:MET:HB3	1:B:132:MET:HE3	1.63	0.81

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:SER:HB3	1:F:303:THR:HB	1.63	0.80
1:D:139:VAL:HA	1:D:165:ILE:HD13	1.64	0.79
1:A:208:ILE:HG21	1:A:247:VAL:HG21	1.62	0.78
1:E:285:CYS:HB3	1:E:289:ILE:HD11	1.65	0.78
2:I:43:ILE:HD11	2:I:76:TYR:HB3	1.65	0.78
1:D:158:GLY:O	1:D:159:VAL:HG13	1.82	0.78
1:E:260:ALA:HB1	1:E:267:LEU:HD11	1.65	0.78
2:K:130:LEU:HD13	2:K:335:LEU:HD11	1.65	0.78
2:H:157:TYR:CE2	2:H:180:MET:CE	2.66	0.78
1:A:208:ILE:HG23	1:A:247:VAL:HG23	1.64	0.77
1:B:250:ILE:HG22	1:B:254:ARG:HG3	1.64	0.77
1:C:31:PHE:HB2	1:C:56:ASP:HA	1.67	0.76
2:H:157:TYR:HD2	2:H:180:MET:HE3	0.96	0.76
1:B:192:ILE:CD1	1:B:253:GLU:HG2	2.15	0.76
1:B:107:GLU:HB3	1:B:134:VAL:HG12	1.66	0.76
2:I:176:LEU:HD23	2:I:176:LEU:C	2.06	0.76
2:J:196:TYR:HD1	2:J:260:LEU:CD2	1.99	0.76
1:B:223:PHE:CD1	1:B:255:PHE:CD1	2.74	0.76
1:B:120:THR:HA	1:B:132:MET:SD	2.25	0.75
1:D:5:ILE:HG21	1:D:101:HIS:ND1	2.01	0.75
1:C:158:GLY:O	1:C:181:ALA:HB2	1.87	0.74
1:E:9:VAL:HG13	1:E:340:TRP:NE1	2.01	0.74
2:J:202:SER:HB3	2:J:238:ALA:HB3	1.70	0.73
1:A:5:ILE:HG21	1:A:100:GLU:O	1.87	0.73
1:B:250:ILE:CG2	1:B:254:ARG:HG2	2.20	0.72
1:D:164:PRO:HG3	1:D:174:ALA:HB3	1.70	0.72
2:J:196:TYR:HD1	2:J:260:LEU:HD21	1.53	0.72
1:B:105:LEU:HD11	1:B:123:MET:HE3	1.70	0.72
1:B:223:PHE:CE1	1:B:255:PHE:CE1	2.77	0.72
1:B:285:CYS:HB3	1:B:289:ILE:HD11	1.73	0.71
2:H:157:TYR:CE2	2:H:180:MET:HE3	2.22	0.71
1:B:24:ASP:HB2	1:B:340:TRP:HH2	1.56	0.71
2:I:28:ILE:HG22	2:I:32:LEU:CD1	2.21	0.71
1:E:212:ILE:O	1:E:212:ILE:CG2	2.34	0.70
1:A:120:THR:HA	1:A:132:MET:SD	2.31	0.70
2:J:196:TYR:CD1	2:J:260:LEU:CD2	2.73	0.70
2:J:355:GLN:O	2:J:359:HIS:CD2	2.44	0.70
2:I:153:VAL:HB	2:I:180:MET:HG3	1.72	0.69
1:F:35:VAL:HG11	1:F:37:ARG:NH2	2.08	0.69
1:B:223:PHE:CD1	1:B:255:PHE:CE1	2.80	0.69
2:J:355:GLN:O	2:J:359:HIS:CE1	2.46	0.68

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:CG2	1:A:67:LEU:CD2	2.71	0.68
1:B:223:PHE:CE1	1:B:255:PHE:HE1	2.11	0.68
2:H:157:TYR:CE2	2:H:180:MET:HE1	2.27	0.68
1:B:188:TYR:CE1	1:B:266:PHE:O	2.46	0.68
1:B:120:THR:HG22	1:B:362:TYR:HE2	1.59	0.68
1:B:188:TYR:OH	1:B:266:PHE:HB3	1.94	0.67
1:D:105:LEU:HB2	1:D:134:VAL:HG12	1.76	0.67
2:I:28:ILE:HG22	2:I:32:LEU:HD13	1.76	0.67
1:D:158:GLY:O	1:D:159:VAL:CG1	2.43	0.67
1:F:158:GLY:O	1:F:181:ALA:HB2	1.94	0.67
2:I:28:ILE:O	2:I:32:LEU:HD13	1.94	0.67
1:A:189:LEU:HD12	1:A:192:ILE:HD11	1.77	0.67
1:B:105:LEU:CD2	1:B:123:MET:CE	2.60	0.66
1:C:159:VAL:HG11	1:C:177:ARG:NH1	2.09	0.66
2:J:164:GLU:HB3	2:J:166:LYS:HE3	1.77	0.66
1:B:250:ILE:CG2	1:B:254:ARG:CG	2.73	0.66
1:B:250:ILE:HG21	1:B:254:ARG:HG2	1.76	0.66
1:F:104:LEU:HD12	1:F:347:ALA:HB2	1.77	0.65
1:A:212:ILE:HG23	1:A:216:LEU:HD12	1.79	0.64
1:E:164:PRO:HD2	1:E:175:ILE:HG22	1.79	0.64
1:B:151:ILE:HG23	1:B:297:THR:HA	1.78	0.64
1:B:50:LYS:N	1:B:53:TYR:HH	1.96	0.64
1:B:153:MET:HG2	1:B:162:THR:HG22	1.77	0.64
1:A:192:ILE:HD12	1:A:253:GLU:HB3	1.80	0.64
2:J:147:ARG:HH11	2:J:159:VAL:HG12	1.63	0.64
2:J:355:GLN:O	2:J:359:HIS:ND1	2.30	0.64
1:B:215:LYS:O	1:B:215:LYS:HG2	1.97	0.64
1:F:303:THR:O	1:F:303:THR:HG22	1.99	0.63
1:F:80:ASP:O	1:F:83:GLU:HG3	1.99	0.62
1:A:113:LYS:HA	1:A:116:ARG:HG3	1.81	0.62
1:F:81:ASP:HA	1:F:84:LYS:HD2	1.81	0.62
1:B:223:PHE:CD1	1:B:255:PHE:HD1	2.16	0.62
1:B:223:PHE:HD1	1:B:255:PHE:CD1	2.17	0.62
1:C:303:THR:HG22	1:C:303:THR:O	2.00	0.62
2:I:142:VAL:HG21	2:I:290:GLN:HB3	1.82	0.61
1:B:140:LEU:HD22	1:B:346:LEU:HD12	1.82	0.61
1:B:182:GLY:HA2	1:B:185:LEU:HD12	1.81	0.61
1:C:21:PHE:HB2	1:C:24:ASP:OD2	2.01	0.61
1:B:223:PHE:HD1	1:B:255:PHE:HD1	1.49	0.60
2:H:201:ARG:HA	2:H:258:ALA:HB1	1.83	0.60
2:I:176:LEU:O	2:I:180:MET:HB2	2.01	0.60

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:LEU:HA	1:F:192:ILE:HG12	1.83	0.59
2:J:196:TYR:CD1	2:J:260:LEU:HD22	2.37	0.59
1:F:120:THR:HA	1:F:132:MET:SD	2.42	0.59
1:A:72:GLU:OE2	1:A:73:HIS:HD2	1.85	0.59
1:C:204:ALA:O	1:C:205:GLU:C	2.41	0.59
1:F:24:ASP:HB2	1:F:340:TRP:HH2	1.66	0.59
1:C:202:THR:CG2	1:C:203:THR:N	2.44	0.59
1:B:119:MET:CB	1:B:132:MET:HE3	2.31	0.58
1:A:72:GLU:OE2	1:A:73:HIS:CD2	2.56	0.58
1:C:186:THR:CG2	1:C:209:VAL:HG23	2.30	0.58
1:A:227:MET:HG2	1:C:324:THR:HG21	1.85	0.58
1:D:219:VAL:HG22	1:D:258:PRO:HB3	1.85	0.58
2:H:212:ALA:HB1	2:H:228:LEU:HD22	1.84	0.58
2:J:200:ASP:HB3	2:J:239:ILE:HG23	1.85	0.58
1:C:136:ILE:HG22	1:C:138:ALA:H	1.67	0.58
2:K:149:SER:HA	2:K:277:LYS:NZ	2.18	0.58
1:A:160:THR:HG22	1:A:180:LEU:O	2.04	0.57
1:F:158:GLY:O	1:F:181:ALA:CB	2.52	0.57
2:I:260:LEU:HA	2:I:309:GLU:HG2	1.85	0.57
2:K:156:GLU:OE1	2:K:156:GLU:N	2.36	0.57
2:I:177:SER:HB2	2:I:263:THR:HB	1.86	0.57
2:K:147:ARG:HH12	2:K:160:THR:HA	1.69	0.57
2:J:229:VAL:HB	2:J:230:PRO:HD2	1.86	0.57
2:K:259:SER:OG	2:K:260:LEU:N	2.38	0.57
2:J:54:LEU:HD11	2:J:86:PHE:HE1	1.70	0.56
1:B:192:ILE:HA	1:B:195:GLU:HB2	1.86	0.56
1:D:156:GLY:O	1:D:181:ALA:HB1	2.05	0.56
1:B:120:THR:HG22	1:B:362:TYR:CD2	2.39	0.56
1:D:151:ILE:HG21	1:D:282:ILE:HD11	1.87	0.56
1:B:119:MET:HB3	1:B:132:MET:CE	2.35	0.56
1:B:189:LEU:CD1	1:B:192:ILE:HD11	2.34	0.56
1:D:155:SER:OG	1:D:160:THR:HG23	2.06	0.56
1:A:35:VAL:CG2	1:A:85:ILE:CD1	2.84	0.55
1:E:9:VAL:CG1	1:E:340:TRP:NE1	2.70	0.55
1:C:259:GLU:C	1:C:261:LEU:N	2.57	0.55
2:K:273:ASP:OD2	2:K:277:LYS:NZ	2.37	0.55
1:F:189:LEU:O	1:F:193:LEU:HB2	2.06	0.55
1:C:139:VAL:HA	1:C:165:ILE:HD13	1.88	0.55
1:A:164:PRO:HG2	1:A:174:ALA:HB3	1.89	0.55
1:F:155:SER:CB	1:F:303:THR:HB	2.36	0.55
2:K:268:MET:HG3	2:K:319:LEU:HD13	1.87	0.55

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:275:ILE:HA	2:K:284:ILE:HD11	1.89	0.54
1:D:5:ILE:CG2	1:D:101:HIS:CE1	2.91	0.54
1:D:91:TYR:O	1:D:95:ARG:HA	2.07	0.54
1:E:180:LEU:HD11	1:E:267:LEU:HD13	1.90	0.54
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.88	0.54
2:K:268:MET:HE1	2:K:271:LEU:HD12	1.89	0.54
2:H:28:ILE:HA	2:H:31:SER:HB2	1.88	0.54
1:B:73:HIS:HB3	1:B:177:ARG:HH22	1.71	0.54
1:C:137:GLN:HG2	1:C:339:VAL:HG11	1.90	0.54
1:D:136:ILE:HB	1:D:139:VAL:HG23	1.89	0.54
2:I:187:LEU:HD23	2:I:190:LYS:HD2	1.90	0.54
1:D:145:SER:HB2	1:D:147:ARG:HH11	1.71	0.54
1:D:21:PHE:O	1:D:22:ALA:C	2.47	0.53
1:D:155:SER:HB3	1:D:303:THR:OG1	2.07	0.53
1:E:185:LEU:O	1:E:188:TYR:HB3	2.08	0.53
1:F:109:PRO:HB3	1:F:175:ILE:HD13	1.89	0.53
1:B:223:PHE:CE1	1:B:255:PHE:CD1	2.97	0.53
1:B:105:LEU:HD11	1:B:123:MET:CE	2.39	0.53
2:K:141:SER:HB3	2:K:144:ASN:HB2	1.91	0.53
1:B:155:SER:HB2	1:B:303:THR:HB	1.90	0.53
1:B:213:LYS:HD3	1:B:240:TYR:CD2	2.44	0.53
1:B:119:MET:CB	1:B:132:MET:CE	2.87	0.53
1:B:194:THR:HG22	1:B:194:THR:O	2.09	0.53
1:D:242:LEU:HD13	1:D:246:GLN:HB3	1.90	0.53
1:C:155:SER:CB	1:C:303:THR:HB	2.32	0.52
1:B:188:TYR:CG	1:B:267:LEU:HD11	2.44	0.52
1:D:242:LEU:O	1:D:245:GLY:N	2.38	0.52
1:E:103:VAL:HG11	1:E:123:MET:SD	2.50	0.52
1:E:118:LYS:HA	1:E:121:GLN:HG2	1.90	0.52
1:A:178:LEU:HD11	1:A:271:SER:HB3	1.90	0.52
2:J:65:GLU:O	2:J:69:LYS:HG3	2.10	0.52
1:A:133:TYR:CE2	1:A:355:MET:HG3	2.44	0.52
1:A:357:ILE:HD11	1:A:374:CYS:SG	2.50	0.52
1:B:11:ASP:HA	1:B:106:THR:OG1	2.10	0.52
1:B:345:ILE:O	1:B:349:LEU:HG	2.10	0.52
1:D:159:VAL:CG2	1:D:161:HIS:NE2	2.73	0.52
1:E:264:PRO:C	1:E:266:PHE:H	2.13	0.52
1:F:70:PRO:HG3	1:F:85:ILE:HD11	1.91	0.52
1:B:91:TYR:O	1:B:95:ARG:HA	2.10	0.52
1:B:185:LEU:HD23	1:B:260:ALA:HB3	1.92	0.52
1:B:360:GLN:HA	1:B:363:ASP:HB2	1.92	0.52

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:THR:HG21	1:E:370:VAL:HB	1.92	0.52
1:B:163:VAL:HG13	1:B:175:ILE:HG12	1.91	0.52
1:D:35:VAL:HG12	1:D:68:LYS:HB2	1.91	0.52
1:C:242:LEU:HD12	1:C:246:GLN:HB3	1.93	0.51
1:D:113:LYS:H	1:D:113:LYS:HD2	1.75	0.51
1:E:351:THR:HG22	2:K:30:LEU:HD13	1.92	0.51
1:B:189:LEU:HD12	1:B:192:ILE:CD1	2.35	0.51
1:D:193:LEU:HD21	1:D:250:ILE:HG23	1.91	0.51
1:B:185:LEU:HD21	1:B:261:LEU:HG	1.92	0.51
1:F:189:LEU:HD12	1:F:192:ILE:HD11	1.92	0.51
1:A:20:GLY:HA2	1:A:28:ARG:H	1.76	0.51
1:B:192:ILE:HD11	1:B:253:GLU:HB3	1.91	0.51
1:A:104:LEU:HD12	1:A:133:TYR:HB3	1.93	0.51
1:C:275:HIS:CD2	1:C:276:GLU:HG3	2.46	0.51
1:D:5:ILE:HG21	1:D:101:HIS:CE1	2.45	0.51
2:J:146:LEU:O	2:J:150:TYR:N	2.43	0.51
2:J:260:LEU:HA	2:J:309:GLU:OE2	2.11	0.51
2:K:212:ALA:O	2:K:229:VAL:HG22	2.10	0.51
1:A:35:VAL:HG23	1:A:85:ILE:CD1	2.41	0.51
1:A:300:SER:HA	1:A:335:ARG:HB2	1.93	0.51
2:I:120:ARG:HH22	2:I:256:PHE:HB3	1.76	0.51
2:K:120:ARG:NH1	2:K:217:MET:HG2	2.25	0.51
2:I:254:THR:HG21	2:I:308:SER:HB2	1.92	0.50
2:H:360:HIS:HA	2:H:363:GLN:HB2	1.94	0.50
2:I:180:MET:HB3	2:I:181:LEU:HD23	1.92	0.50
2:J:259:SER:HB2	2:J:305:HIS:CG	2.47	0.50
1:A:23:GLY:H	1:A:344:SER:HB2	1.76	0.50
1:A:176:LEU:HD11	1:A:284:LYS:HZ1	1.76	0.50
2:H:260:LEU:HA	2:H:309:GLU:HG2	1.93	0.50
2:J:68:GLU:HG2	2:J:342:PHE:CD1	2.46	0.50
1:F:218:TYR:O	1:F:255:PHE:HA	2.11	0.50
1:C:186:THR:HG23	1:C:209:VAL:CG2	2.35	0.50
1:C:189:LEU:HD23	1:C:209:VAL:HB	1.92	0.50
2:H:157:TYR:HE2	2:H:180:MET:HE1	1.75	0.50
2:I:221:SER:O	2:I:222:PRO:C	2.49	0.50
2:I:232:ARG:HE	2:I:234:VAL:HG22	1.77	0.50
1:B:136:ILE:HG22	1:B:138:ALA:H	1.76	0.50
1:A:170:ALA:H	1:A:375:PHE:HZ	1.57	0.49
1:A:299:LEU:HD13	1:A:309:ILE:HG23	1.94	0.49
1:B:213:LYS:HD2	1:B:250:ILE:HG12	1.94	0.49
1:F:5:ILE:HD12	1:F:102:PRO:HD3	1.93	0.49

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:GLU:OE1	1:D:99:GLU:N	2.42	0.49
2:J:259:SER:O	2:J:309:GLU:HB3	2.12	0.49
2:J:256:PHE:HB2	2:J:258:ALA:H	1.76	0.49
2:H:212:ALA:O	2:H:229:VAL:HG22	2.13	0.49
2:I:129:HIS:CD2	2:I:335:LEU:HD13	2.47	0.49
1:C:240:TYR:CE1	1:C:248:ILE:HG12	2.48	0.49
2:K:199:LYS:HE2	2:K:259:SER:OG	2.12	0.49
2:K:361:GLU:HG2	2:K:362:LEU:N	2.27	0.49
1:C:10:ILE:HD12	1:C:89:THR:HG21	1.94	0.49
1:A:18:LYS:HE2	1:A:337:TYR:HD1	1.76	0.49
1:D:212:ILE:HG23	1:D:216:LEU:HD12	1.94	0.49
1:E:59:GLN:O	1:E:60:SER:C	2.50	0.49
1:F:5:ILE:O	1:F:5:ILE:HG13	2.13	0.49
1:A:185:LEU:HD11	1:A:261:LEU:HG	1.95	0.49
1:D:70:PRO:HB3	1:D:81:ASP:OD1	2.13	0.49
1:D:158:GLY:C	1:D:159:VAL:HG13	2.32	0.49
1:E:89:THR:HA	1:E:93:GLU:HB2	1.95	0.48
1:C:120:THR:HA	1:C:132:MET:SD	2.53	0.48
1:C:153:MET:HG2	1:C:162:THR:HG22	1.95	0.48
1:F:264:PRO:HB2	1:F:269:MET:HB2	1.95	0.48
2:I:176:LEU:HD23	2:I:177:SER:CB	2.42	0.48
1:A:20:GLY:CA	1:A:28:ARG:H	2.26	0.48
2:I:232:ARG:H	2:I:232:ARG:HG2	1.29	0.48
1:E:102:PRO:HB3	1:E:131:ALA:HB3	1.94	0.48
1:F:313:MET:O	1:F:317:ILE:HG22	2.13	0.48
2:J:259:SER:HB2	2:J:305:HIS:ND1	2.28	0.48
2:K:172:LYS:HA	2:K:175:ILE:HG22	1.96	0.48
1:B:312:ARG:O	1:B:313:MET:C	2.49	0.48
2:K:358:MET:HA	2:K:361:GLU:OE1	2.13	0.48
1:C:212:ILE:HG23	1:C:216:LEU:HD12	1.94	0.48
2:J:229:VAL:HB	2:J:230:PRO:CD	2.44	0.48
1:D:12:ASN:HD21	1:D:86:TRP:HE1	1.60	0.48
2:I:175:ILE:O	2:I:176:LEU:C	2.50	0.48
2:J:43:ILE:HD12	2:J:71:TYR:HD1	1.78	0.48
2:I:256:PHE:O	2:I:256:PHE:CD2	2.67	0.47
2:I:345:ALA:O	2:I:349:VAL:HG23	2.14	0.47
1:A:273:GLY:C	1:A:275:HIS:N	2.67	0.47
2:I:32:LEU:HD12	2:I:45:LEU:HD23	1.96	0.47
2:J:85:ASP:OD1	2:J:88:LYS:NZ	2.47	0.47
1:A:72:GLU:O	1:A:73:HIS:C	2.52	0.47
1:D:105:LEU:HD11	1:D:123:MET:SD	2.54	0.47

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:278:HIS:O	2:K:284:ILE:HD12	2.15	0.47
2:K:284:ILE:HA	2:K:287:LYS:HB2	1.95	0.47
1:A:124:PHE:O	1:A:128:ASN:HA	2.15	0.47
1:A:109:PRO:HG2	1:A:163:VAL:HG21	1.97	0.47
1:D:188:TYR:O	1:D:192:ILE:HG12	2.14	0.47
1:C:148:THR:HG1	2:I:359:HIS:CE1	2.31	0.47
1:E:58:ALA:O	1:E:67:LEU:HD21	2.15	0.47
1:F:222:ASP:HB3	1:F:225:GLN:HB3	1.95	0.47
1:F:314:GLN:HG2	1:F:329:ILE:HG13	1.97	0.47
2:H:358:MET:C	2:H:360:HIS:N	2.66	0.47
2:I:184:ASN:H	2:I:187:LEU:HG	1.80	0.47
1:B:333:PRO:C	1:B:335:ARG:H	2.18	0.47
2:K:120:ARG:HH11	2:K:217:MET:HG2	1.80	0.47
1:B:143:TYR:CE2	1:B:346:LEU:CD1	2.84	0.47
1:D:12:ASN:ND2	1:D:86:TRP:HE1	2.13	0.47
2:J:129:HIS:CE1	2:J:335:LEU:HD13	2.50	0.47
1:B:192:ILE:HB	1:B:253:GLU:HG2	1.97	0.46
1:B:275:HIS:HA	1:B:313:MET:SD	2.56	0.46
1:F:186:THR:O	1:F:187:ASP:HB2	2.15	0.46
2:H:150:TYR:CD2	2:H:159:VAL:HG22	2.51	0.46
1:A:190:MET:HG2	1:A:209:VAL:HG11	1.97	0.46
1:B:143:TYR:CD2	1:B:346:LEU:CD1	2.73	0.46
2:I:119:ARG:HG2	2:I:255:PRO:HD3	1.97	0.46
1:B:120:THR:CG2	1:B:362:TYR:CD2	2.99	0.46
1:D:287:VAL:HG12	1:D:287:VAL:O	2.15	0.46
2:I:126:TYR:OH	2:I:335:LEU:HB2	2.14	0.46
2:J:212:ALA:HB1	2:J:228:LEU:HD23	1.97	0.46
1:D:194:THR:HA	1:D:198:TYR:O	2.14	0.46
1:E:352:PHE:C	1:E:354:GLN:H	2.18	0.46
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.97	0.46
2:J:247:TYR:CD2	2:J:258:ALA:HB1	2.50	0.46
1:A:332:PRO:HD2	1:A:335:ARG:HB3	1.97	0.46
1:B:98:PRO:HB2	1:B:129:THR:HG22	1.97	0.46
1:C:192:ILE:HG13	1:C:253:GLU:HG2	1.98	0.46
1:E:264:PRO:C	1:E:266:PHE:N	2.68	0.46
2:I:63:PHE:O	2:I:67:ILE:HG12	2.15	0.46
2:I:356:SER:HA	2:I:359:HIS:HB3	1.98	0.46
1:E:151:ILE:HG23	1:E:297:THR:HG23	1.98	0.46
2:I:112:ASN:O	2:I:116:ASN:HB2	2.16	0.46
2:I:176:LEU:CD2	2:I:177:SER:HB3	2.46	0.46
1:B:342:GLY:O	1:B:346:LEU:HG	2.15	0.46

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:GLN:HA	1:D:339:VAL:HG13	1.98	0.46
2:H:117:GLU:HA	2:H:120:ARG:HG3	1.98	0.46
2:H:130:LEU:O	2:H:134:ILE:HG12	2.16	0.46
2:J:330:LEU:HD23	2:J:330:LEU:HA	1.78	0.46
1:D:152:VAL:HG22	1:D:298:VAL:HG22	1.96	0.45
1:D:263:GLN:C	1:D:265:SER:H	2.19	0.45
1:C:12:ASN:HD21	1:C:86:TRP:HE1	1.62	0.45
2:I:94:LEU:HB3	2:I:95:SER:H	1.38	0.45
2:I:165:ILE:O	2:I:167:THR:N	2.48	0.45
1:A:272:CYS:HB3	1:A:276:GLU:HB2	1.98	0.45
1:C:54:VAL:HG21	1:C:84:LYS:HB3	1.98	0.45
1:C:208:ILE:HG22	1:C:208:ILE:O	2.15	0.45
1:A:112:PRO:O	1:A:115:ASN:HB2	2.16	0.45
1:B:114:ALA:O	1:B:118:LYS:N	2.46	0.45
1:E:120:THR:O	1:E:124:PHE:HB2	2.16	0.45
2:K:140:LEU:HD13	2:K:140:LEU:HA	1.82	0.45
1:E:9:VAL:CG1	1:E:340:TRP:CE2	3.00	0.45
1:E:117:GLU:HG3	1:E:371:HIS:CE1	2.52	0.45
1:E:217:CYS:SG	1:E:254:ARG:HA	2.57	0.45
1:F:151:ILE:HG23	1:F:297:THR:HG23	1.99	0.45
2:H:157:TYR:CD2	2:H:180:MET:HE1	2.34	0.45
2:I:284:ILE:HG12	2:I:288:VAL:HG23	1.98	0.45
2:J:130:LEU:HD23	2:J:297:SER:HB3	1.99	0.45
1:B:163:VAL:HG22	1:B:175:ILE:HG23	1.98	0.45
2:J:356:SER:O	2:J:359:HIS:HB2	2.17	0.45
1:C:259:GLU:C	1:C:261:LEU:H	2.19	0.45
2:I:285:GLU:O	2:I:289:ASN:HB2	2.17	0.45
1:A:312:ARG:O	1:A:313:MET:C	2.52	0.45
1:A:350:SER:O	1:A:353:GLN:HB2	2.17	0.45
1:B:265:SER:C	1:B:268:GLY:H	2.19	0.45
2:I:32:LEU:HD21	2:I:102:LEU:CD2	2.47	0.45
2:K:285:GLU:HG3	2:K:328:ILE:HG23	1.99	0.45
1:A:143:TYR:HD1	1:A:143:TYR:HA	1.71	0.45
1:D:159:VAL:HG21	1:D:161:HIS:NE2	2.32	0.45
2:J:209:THR:OG1	2:J:236:LYS:HG2	2.17	0.45
1:B:87:HIS:O	1:B:91:TYR:HB2	2.17	0.45
1:D:242:LEU:HD11	1:D:248:ILE:HD11	1.99	0.45
1:F:208:ILE:H	1:F:208:ILE:HG12	1.56	0.45
2:H:132:SER:HA	2:H:135:LYS:HB2	1.98	0.45
2:I:199:LYS:HE3	2:I:259:SER:HB2	1.98	0.45
2:J:239:ILE:HG13	2:J:257:VAL:HG12	1.99	0.45

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:GLU:O	1:B:277:THR:C	2.52	0.44
1:B:335:ARG:HA	1:B:338:SER:HB3	1.99	0.44
1:D:73:HIS:HB3	1:D:177:ARG:NH2	2.32	0.44
1:D:335:ARG:H	1:D:335:ARG:HG2	1.59	0.44
2:H:213:ASN:HA	2:H:214:PRO:HD3	1.87	0.44
1:A:6:ALA:O	1:A:102:PRO:HD2	2.17	0.44
1:C:189:LEU:HA	1:C:192:ILE:HG12	1.99	0.44
1:D:275:HIS:H	1:D:275:HIS:CD2	2.34	0.44
1:D:113:LYS:HD2	1:D:113:LYS:N	2.31	0.44
1:E:142:LEU:HD13	1:E:152:VAL:HG22	1.98	0.44
2:H:200:ASP:OD1	2:H:200:ASP:N	2.51	0.44
2:J:54:LEU:HD11	2:J:86:PHE:CE1	2.49	0.44
1:B:136:ILE:HB	1:B:139:VAL:HG23	2.00	0.44
1:B:349:LEU:HD23	1:B:349:LEU:HA	1.88	0.44
1:D:159:VAL:HG23	1:D:161:HIS:NE2	2.32	0.44
2:J:196:TYR:N	2:J:197:PRO:HD2	2.32	0.44
1:E:303:THR:C	1:E:305:MET:H	2.21	0.44
1:E:9:VAL:HG13	1:E:9:VAL:O	2.18	0.44
1:F:189:LEU:HG	1:F:193:LEU:HD12	1.99	0.44
2:H:196:TYR:O	2:H:199:LYS:HG3	2.18	0.44
1:D:73:HIS:HA	1:D:159:VAL:HG13	1.99	0.44
1:E:99:GLU:H	1:E:99:GLU:HG2	1.50	0.44
1:E:113:LYS:HB3	1:E:113:LYS:HE3	1.78	0.44
2:H:28:ILE:HG22	2:H:32:LEU:HG	2.00	0.44
1:B:83:GLU:HG2	1:B:122:ILE:HD13	2.00	0.44
1:B:180:LEU:HD21	1:B:261:LEU:HA	1.98	0.44
1:D:37:ARG:HB2	1:D:37:ARG:NH1	2.32	0.44
1:E:136:ILE:HB	1:E:139:VAL:HG23	1.99	0.44
1:A:163:VAL:HG13	1:A:175:ILE:HG12	2.00	0.43
1:B:189:LEU:HD13	1:B:257:CYS:HB2	2.00	0.43
1:F:275:HIS:CD2	1:F:276:GLU:HG3	2.53	0.43
1:A:192:ILE:HB	1:A:253:GLU:HG2	1.99	0.43
1:C:341:ILE:O	1:C:345:ILE:HG13	2.17	0.43
2:I:213:ASN:HD21	2:I:227:ASN:HB3	1.82	0.43
1:A:124:PHE:CE2	1:A:132:MET:HG2	2.54	0.43
1:B:251:GLY:C	1:B:253:GLU:H	2.20	0.43
1:F:213:LYS:HE2	1:F:213:LYS:HB3	1.88	0.43
1:D:163:VAL:HG13	1:D:175:ILE:HG12	2.01	0.43
2:K:144:ASN:O	2:K:147:ARG:HB3	2.19	0.43
2:K:353:THR:O	2:K:357:ALA:N	2.44	0.43
1:A:78:ASN:HD22	1:A:78:ASN:HA	1.59	0.43

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PRO:HG2	1:A:174:ALA:CB	2.47	0.43
1:C:171:LEU:O	1:C:175:ILE:HG13	2.18	0.43
2:K:155:PRO:O	2:K:158:ALA:HB2	2.19	0.43
1:D:39:ARG:H	1:D:65:LEU:N	2.17	0.43
1:E:37:ARG:O	1:E:38:PRO:C	2.56	0.43
1:E:345:ILE:O	1:E:349:LEU:HG	2.18	0.43
1:F:5:ILE:CD1	1:F:102:PRO:HD3	2.48	0.43
2:I:331:ASN:HD22	2:I:331:ASN:HA	1.53	0.43
2:J:101:ARG:O	2:J:105:VAL:HG23	2.19	0.43
1:B:154:ASP:O	1:B:160:THR:HA	2.19	0.43
1:D:189:LEU:HD23	1:D:209:VAL:HG13	2.00	0.43
2:I:196:TYR:O	2:I:199:LYS:HG3	2.19	0.43
1:C:193:LEU:HD21	1:C:250:ILE:HG23	2.01	0.43
1:C:261:LEU:O	1:C:273:GLY:HA2	2.19	0.43
2:H:121:LEU:O	2:H:125:LEU:HG	2.19	0.43
2:H:176:LEU:HD23	2:H:299:TYR:CE1	2.53	0.43
2:H:28:ILE:C	2:H:30:LEU:N	2.70	0.43
2:K:123:GLU:HB3	2:K:300:ILE:HG21	2.00	0.43
2:K:356:SER:O	2:K:359:HIS:ND1	2.52	0.43
1:D:11:ASP:HA	1:D:106:THR:OG1	2.19	0.42
1:F:96:VAL:HB	1:F:101:HIS:CE1	2.53	0.42
2:H:63:PHE:HE2	2:H:83:ILE:HA	1.84	0.42
2:I:220:ASN:O	2:I:221:SER:C	2.56	0.42
2:J:256:PHE:HB3	2:J:257:VAL:H	1.30	0.42
1:B:276:GLU:C	1:B:278:THR:N	2.71	0.42
1:F:186:THR:C	1:F:188:TYR:H	2.21	0.42
2:K:175:ILE:HD11	2:K:291:ILE:HG23	2.01	0.42
1:E:219:VAL:HG22	1:E:258:PRO:CB	2.50	0.42
2:J:43:ILE:HD12	2:J:71:TYR:CD1	2.54	0.42
2:K:202:SER:HB2	2:K:240:ASN:HB2	2.01	0.42
2:K:214:PRO:HB2	2:K:301:LYS:O	2.20	0.42
2:I:72:PHE:HA	2:I:119:ARG:HH12	1.83	0.42
2:K:200:ASP:OD1	2:K:247:TYR:HB3	2.19	0.42
1:D:287:VAL:O	1:D:287:VAL:CG1	2.68	0.42
1:E:120:THR:CG2	1:E:370:VAL:HB	2.49	0.42
1:E:354:GLN:HE21	1:E:354:GLN:HB2	1.70	0.42
1:F:292:ASP:O	1:F:296:ASN:HB2	2.19	0.42
2:H:68:GLU:O	2:H:69:LYS:C	2.55	0.42
2:I:176:LEU:HG	2:I:270:VAL:HG21	2.02	0.42
2:K:77:LYS:HG3	2:K:81:GLU:OE2	2.20	0.42
1:F:281:SER:OG	1:F:282:ILE:N	2.53	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:ASP:O	1:F:289:ILE:HG12	2.20	0.42
1:F:303:THR:O	1:F:303:THR:CG2	2.66	0.42
2:I:212:ALA:O	2:I:229:VAL:HG22	2.19	0.42
2:J:23:LYS:HE3	2:J:23:LYS:HB3	1.91	0.42
2:J:260:LEU:HA	2:J:309:GLU:CD	2.40	0.42
2:K:149:SER:HA	2:K:277:LYS:HZ3	1.83	0.42
1:B:255:PHE:O	1:B:259:GLU:HB2	2.19	0.42
1:B:260:ALA:HB1	1:B:267:LEU:HD13	2.02	0.42
1:C:251:GLY:O	1:C:252:ASN:HB2	2.20	0.42
1:F:317:ILE:HG21	1:F:329:ILE:HD11	2.02	0.42
2:J:259:SER:HB2	2:J:305:HIS:CB	2.49	0.42
1:A:16:MET:HB2	1:A:16:MET:HE2	1.90	0.42
1:C:286:ASP:O	1:C:290:ARG:HG3	2.20	0.42
1:E:14:SER:CB	1:E:158:GLY:HA3	2.50	0.42
1:F:219:VAL:HG12	1:F:258:PRO:HB3	2.02	0.42
2:I:32:LEU:CD1	2:I:45:LEU:HD23	2.50	0.42
2:I:34:SER:C	2:I:36:LYS:N	2.73	0.42
2:J:95:SER:OG	2:J:98:VAL:HG23	2.20	0.42
2:K:364:GLU:O	2:K:368:ASN:N	2.53	0.42
1:E:355:MET:HG3	2:K:358:MET:SD	2.60	0.41
2:J:296:ILE:HG12	2:J:310:VAL:HG11	2.02	0.41
1:D:70:PRO:HG2	1:D:85:ILE:HD11	2.02	0.41
1:F:339:VAL:HG13	1:F:340:TRP:N	2.36	0.41
2:I:39:GLU:HA	2:I:109:LEU:HD13	2.01	0.41
1:A:34:ILE:HG22	1:A:67:LEU:HD23	2.03	0.41
1:C:251:GLY:C	1:C:253:GLU:H	2.23	0.41
1:C:262:PHE:HE2	1:C:313:MET:HG3	1.85	0.41
2:H:356:SER:HA	2:H:359:HIS:HB2	2.02	0.41
2:J:247:TYR:CE2	2:J:258:ALA:HB1	2.55	0.41
1:A:191:LYS:O	1:A:194:THR:HB	2.20	0.41
1:D:8:LEU:HD13	1:D:90:PHE:HE1	1.85	0.41
1:E:213:LYS:HE3	1:E:214:GLU:OE1	2.19	0.41
1:F:190:MET:O	1:F:194:THR:HG23	2.21	0.41
2:H:256:PHE:O	2:H:256:PHE:CG	2.73	0.41
1:A:171:LEU:O	1:A:175:ILE:HG13	2.20	0.41
1:E:35:VAL:HG23	1:E:70:PRO:HD3	2.03	0.41
1:F:61:LYS:HB2	1:F:65:LEU:HG	2.03	0.41
2:I:176:LEU:CD2	2:I:177:SER:CB	2.98	0.41
1:A:103:VAL:O	1:A:132:MET:HA	2.21	0.41
1:C:303:THR:O	1:C:303:THR:CG2	2.68	0.41
1:D:136:ILE:HG22	1:D:138:ALA:H	1.84	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:VAL:HG22	1:D:175:ILE:HG23	2.01	0.41
1:E:175:ILE:O	1:E:175:ILE:HG13	2.21	0.41
1:F:142:LEU:HD22	1:F:165:ILE:HD12	2.02	0.41
1:F:155:SER:HB2	1:F:304:THR:HG23	2.03	0.41
2:H:67:ILE:HG23	2:H:79:ALA:HB1	2.01	0.41
1:F:107:GLU:O	1:F:137:GLN:HG3	2.20	0.41
2:H:88:LYS:HA	2:H:91:GLU:HG3	2.02	0.41
1:C:108:ALA:O	1:C:109:PRO:C	2.57	0.41
1:D:87:HIS:O	1:D:91:TYR:N	2.50	0.41
1:E:9:VAL:HG13	1:E:340:TRP:HE1	1.84	0.41
1:E:287:VAL:H	1:E:287:VAL:HG23	1.65	0.41
2:I:221:SER:HB3	2:I:348:TYR:OH	2.21	0.41
1:A:111:ASN:O	1:A:112:PRO:C	2.55	0.41
1:B:213:LYS:H	1:B:213:LYS:HG2	1.17	0.41
1:B:256:ARG:HE	1:B:256:ARG:HB3	1.77	0.41
1:C:155:SER:O	1:C:301:GLY:HA3	2.21	0.41
1:C:278:THR:O	1:C:282:ILE:HG13	2.21	0.41
1:E:228:ALA:C	1:E:230:ALA:H	2.24	0.41
1:E:341:ILE:O	1:E:345:ILE:HG13	2.21	0.41
2:H:342:PHE:O	2:H:346:GLN:HG3	2.20	0.41
2:I:142:VAL:HB	2:I:287:LYS:HB3	2.02	0.41
2:I:228:LEU:HA	2:I:228:LEU:HD23	1.78	0.41
2:J:255:PRO:O	2:J:256:PHE:HB2	2.20	0.41
2:I:153:VAL:O	2:I:154:LYS:C	2.59	0.41
2:J:129:HIS:O	2:J:133:VAL:HG23	2.20	0.41
1:A:72:GLU:C	1:A:74:GLY:N	2.71	0.40
1:D:166:TYR:O	1:D:167:GLU:C	2.59	0.40
2:K:268:MET:HG3	2:K:319:LEU:HD22	2.03	0.40
1:B:32:PRO:HB2	1:B:34:ILE:HG12	2.03	0.40
1:E:37:ARG:HB3	1:E:38:PRO:HD2	2.03	0.40
1:E:110:LEU:HB2	1:E:175:ILE:HD11	2.02	0.40
1:D:350:SER:HA	1:D:353:GLN:HG2	2.04	0.40
1:F:165:ILE:HD13	1:F:165:ILE:HG21	1.77	0.40
2:J:337:ASP:OD1	2:J:339:HIS:ND1	2.53	0.40
1:A:161:HIS:CD2	1:A:177:ARG:HB3	2.56	0.40
1:A:191:LYS:HE2	1:A:191:LYS:HB2	1.89	0.40
1:B:89:THR:O	1:B:94:LEU:HB2	2.20	0.40
1:B:118:LYS:HD2	1:B:118:LYS:HA	1.90	0.40
1:C:186:THR:CG2	1:C:209:VAL:CG2	2.96	0.40
1:D:151:ILE:HD13	1:D:282:ILE:HG13	2.03	0.40
1:E:228:ALA:C	1:E:230:ALA:N	2.75	0.40

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:28:ILE:HG22	2:I:32:LEU:HD11	2.01	0.40
1:B:105:LEU:HD21	1:B:123:MET:HE3	1.83	0.40
1:B:360:GLN:O	1:B:361:GLU:C	2.56	0.40
1:E:113:LYS:H	1:E:113:LYS:HG2	1.69	0.40
1:F:31:PHE:HZ	1:F:89:THR:OG1	2.05	0.40
1:F:109:PRO:HD2	1:F:161:HIS:CD2	2.56	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	310/375 (83%)	292 (94%)	17 (6%)	1 (0%)	41 74
1	B	335/375 (89%)	323 (96%)	12 (4%)	0	100 100
1	C	332/375 (88%)	316 (95%)	16 (5%)	0	100 100
1	D	346/375 (92%)	328 (95%)	18 (5%)	0	100 100
1	E	304/375 (81%)	283 (93%)	21 (7%)	0	100 100
1	F	330/375 (88%)	318 (96%)	12 (4%)	0	100 100
2	H	344/441 (78%)	321 (93%)	23 (7%)	0	100 100
2	I	325/441 (74%)	301 (93%)	24 (7%)	0	100 100
2	J	337/441 (76%)	315 (94%)	21 (6%)	1 (0%)	41 74
2	K	321/441 (73%)	305 (95%)	16 (5%)	0	100 100
All	All	3284/4014 (82%)	3102 (94%)	180 (6%)	2 (0%)	51 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
2	J	214	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	275/318 (86%)	261 (95%)	14 (5%)	24	57
1	B	289/318 (91%)	277 (96%)	12 (4%)	30	62
1	C	292/318 (92%)	282 (97%)	10 (3%)	37	68
1	D	302/318 (95%)	291 (96%)	11 (4%)	35	66
1	E	270/318 (85%)	259 (96%)	11 (4%)	30	62
1	F	287/318 (90%)	275 (96%)	12 (4%)	30	62
2	H	322/408 (79%)	303 (94%)	19 (6%)	19	52
2	I	308/408 (76%)	296 (96%)	12 (4%)	32	64
2	J	317/408 (78%)	308 (97%)	9 (3%)	43	73
2	K	305/408 (75%)	299 (98%)	6 (2%)	55	79
All	All	2967/3540 (84%)	2851 (96%)	116 (4%)	32	64

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	85	ILE
1	A	104	LEU
1	A	141	SER
1	A	143	TYR
1	A	145	SER
1	A	160	THR
1	A	202	THR
1	A	255	PHE
1	A	256	ARG
1	A	303	THR
1	A	349	LEU

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	A	354	GLN
1	A	368	SER
1	B	14	SER
1	B	75	ILE
1	B	85	ILE
1	B	99	GLU
1	B	104	LEU
1	B	145	SER
1	B	185	LEU
1	B	212	ILE
1	B	219	VAL
1	B	241	GLU
1	B	341	ILE
1	B	361	GLU
1	C	27	PRO
1	C	32	PRO
1	C	34	ILE
1	C	105	LEU
1	C	221	LEU
1	C	240	TYR
1	C	248	ILE
1	C	327	ILE
1	C	334	GLU
1	C	337	TYR
1	D	25	ASP
1	D	51	ASP
1	D	56	ASP
1	D	166	TYR
1	D	218	TYR
1	D	229	THR
1	D	234	SER
1	D	250	ILE
1	D	258	PRO
1	D	298	VAL
1	D	334	GLU
1	E	59	GLN
1	E	66	THR
1	E	99	GLU
1	E	129	THR
1	E	169	TYR
1	E	175	ILE
1	E	211	ASP

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	E	226	GLU
1	E	249	THR
1	E	276	GLU
1	E	334	GLU
1	F	56	ASP
1	F	83	GLU
1	F	104	LEU
1	F	208	ILE
1	F	219	VAL
1	F	221	LEU
1	F	309	ILE
1	F	318	THR
1	F	324	THR
1	F	351	THR
1	F	359	LYS
1	F	370	VAL
2	H	49	TYR
2	H	59	GLU
2	H	128	ASP
2	H	160	THR
2	H	161	HIS
2	H	162	GLU
2	H	167	THR
2	H	182	ASN
2	H	183	ASP
2	H	200	ASP
2	H	209	THR
2	H	213	ASN
2	H	220	ASN
2	H	221	SER
2	H	226	ASP
2	H	233	ASP
2	H	257	VAL
2	H	322	ILE
2	H	360	HIS
2	I	28	ILE
2	I	45	LEU
2	I	49	TYR
2	I	176	LEU
2	I	180	MET
2	I	181	LEU
2	I	197	PRO

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
2	I	211	SER
2	I	220	ASN
2	I	315	THR
2	I	331	ASN
2	I	337	ASP
2	J	49	TYR
2	J	116	ASN
2	J	118	SER
2	J	167	THR
2	J	174	PHE
2	J	183	ASP
2	J	216	ILE
2	J	248	SER
2	J	299	TYR
2	K	21	TYR
2	K	49	TYR
2	K	183	ASP
2	K	221	SER
2	K	224	PHE
2	K	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	78	ASN
1	A	161	HIS
1	A	354	GLN
1	B	101	HIS
1	B	121	GLN
1	B	360	GLN
1	D	12	ASN
1	D	252	ASN
1	D	275	HIS
1	E	59	GLN
1	E	371	HIS
2	H	346	GLN
2	H	368	ASN
2	I	74	GLN
2	I	182	ASN
2	I	320	GLN
2	I	331	ASN

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
2	I	346	GLN
2	I	355	GLN
2	I	363	GLN
2	J	355	GLN
2	K	74	GLN
2	K	320	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

For Manuscript Review

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	322/375 (85%)	1.29	77 (23%)	0	0	30, 96, 106, 116	0
1	B	343/375 (91%)	1.00	52 (15%)	2	3	40, 84, 100, 161	0
1	C	342/375 (91%)	0.55	20 (5%)	23	24	30, 43, 57, 75	0
1	D	354/375 (94%)	0.53	18 (5%)	28	28	30, 46, 58, 78	0
1	E	318/375 (84%)	0.68	30 (9%)	8	11	32, 49, 63, 77	0
1	F	338/375 (90%)	0.68	22 (6%)	18	21	38, 52, 62, 92	0
2	H	348/441 (78%)	0.49	18 (5%)	27	28	30, 47, 65, 88	0
2	I	335/441 (75%)	0.56	26 (7%)	13	16	33, 46, 61, 77	0
2	J	343/441 (77%)	0.46	13 (3%)	40	40	27, 43, 59, 75	0
2	K	331/441 (75%)	0.69	31 (9%)	8	11	36, 52, 72, 515	0
All	All	3374/4014 (84%)	0.69	307 (9%)	9	12	27, 50, 98, 515	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	220	ASN	7.1
1	A	271	SER	6.5
1	A	272	CYS	5.9
1	A	159	VAL	5.8
1	C	250	ILE	5.7
1	A	375	PHE	5.0
1	F	63	GLY	5.0
1	B	217	CYS	4.9
1	A	80	ASP	4.6
1	A	220	ALA	4.6
1	A	35	VAL	4.6
1	D	36	GLY	4.5
1	A	309	ILE	4.4

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	24	ASP	4.4
1	B	293	LEU	4.3
1	B	357	ILE	4.3
1	A	33	SER	4.3
2	K	217	MET	4.1
1	E	272	CYS	4.0
1	C	355	MET	4.0
2	I	184	ASN	3.9
1	B	83	GLU	3.9
1	E	23	GLY	3.9
2	H	80	ILE	3.9
1	B	240	TYR	3.8
2	I	363	GLN	3.8
2	I	186	GLU	3.8
1	D	66	THR	3.7
2	K	46	SER	3.7
1	A	132	MET	3.7
2	I	176	LEU	3.7
1	F	10	ILE	3.7
2	J	214	PRO	3.7
1	B	358	SER	3.6
1	F	127	PHE	3.6
1	B	359	LYS	3.6
2	K	275	ILE	3.6
1	A	34	ILE	3.4
1	C	192	ILE	3.4
2	I	177	SER	3.4
2	K	157	TYR	3.4
1	D	56	ASP	3.4
1	E	60	SER	3.4
1	C	134	VAL	3.4
1	A	289	ILE	3.4
2	I	55	GLY	3.4
1	A	143	TYR	3.4
1	C	133	TYR	3.4
2	K	159	VAL	3.3
1	C	56	ASP	3.3
1	A	371	HIS	3.3
1	A	160	THR	3.3
1	A	341	ILE	3.3
1	A	370	VAL	3.3
1	F	12	ASN	3.3

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	32	PRO	3.3
1	B	294	TYR	3.2
2	K	248	SER	3.2
1	A	32	PRO	3.2
1	D	25	ASP	3.2
1	D	135	ALA	3.2
2	H	157	TYR	3.2
2	K	265	TYR	3.2
2	K	206	LEU	3.2
2	H	88	LYS	3.2
1	B	132	MET	3.2
2	K	127	ALA	3.2
2	I	179	VAL	3.1
1	F	106	THR	3.1
2	K	150	TYR	3.1
2	I	310	VAL	3.1
1	E	152	VAL	3.1
1	A	109	PRO	3.1
1	A	357	ILE	3.1
1	D	355	MET	3.1
1	B	166	TYR	3.1
1	C	240	TYR	3.1
2	H	362	LEU	3.0
1	B	127	PHE	3.0
1	E	175	ILE	3.0
1	E	84	LYS	3.0
1	B	353	GLN	3.0
1	A	188	TYR	3.0
1	A	221	LEU	3.0
1	A	327	ILE	3.0
1	A	348	SER	3.0
1	F	122	ILE	3.0
2	J	309	GLU	3.0
1	A	67	LEU	3.0
2	I	206	LEU	3.0
1	E	169	TYR	3.0
1	A	209	VAL	3.0
1	B	178	LEU	3.0
1	A	277	THR	2.9
1	B	355	MET	2.9
1	E	155	SER	2.9
1	B	219	VAL	2.9

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	34	ILE	2.9
2	I	256	PHE	2.9
1	F	132	MET	2.9
1	A	247	VAL	2.9
1	A	285	CYS	2.9
1	A	219	VAL	2.9
1	B	180	LEU	2.9
2	K	271	LEU	2.9
1	A	98	PRO	2.9
1	C	159	VAL	2.9
2	I	169	ASP	2.9
2	K	213	ASN	2.9
1	F	318	THR	2.9
1	F	272	CYS	2.9
2	I	257	VAL	2.9
1	B	33	SER	2.9
1	A	119	MET	2.9
1	A	298	VAL	2.9
1	B	34	ILE	2.9
1	A	307	PRO	2.9
1	F	220	ALA	2.8
2	I	88	LYS	2.8
1	A	105	LEU	2.8
1	B	346	LEU	2.8
1	D	175	ILE	2.8
2	K	237	ILE	2.8
1	A	77	THR	2.8
1	A	94	LEU	2.8
2	K	76	TYR	2.8
2	K	238	ALA	2.8
1	B	92	ASN	2.8
2	K	278	HIS	2.8
1	A	329	ILE	2.8
1	B	299	LEU	2.8
1	D	26	ALA	2.8
1	E	66	THR	2.7
1	E	85	ILE	2.7
1	E	327	ILE	2.7
2	J	45	LEU	2.7
1	A	83	GLU	2.7
2	K	200	ASP	2.7
1	B	98	PRO	2.7

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	129	THR	2.7
1	C	357	ILE	2.7
1	E	344	SER	2.7
1	F	153	MET	2.7
1	A	261	LEU	2.6
1	A	31	PHE	2.6
1	A	153	MET	2.6
1	A	349	LEU	2.6
1	F	90	PHE	2.6
1	A	257	CYS	2.6
2	H	329	LYS	2.6
1	C	204	ALA	2.6
2	H	287	LYS	2.6
1	A	81	ASP	2.6
1	A	288	ASP	2.6
2	K	160	THR	2.6
1	E	129	THR	2.6
1	B	134	VAL	2.6
2	K	252	PRO	2.6
1	B	123	MET	2.6
1	E	82	MET	2.6
1	B	317	ILE	2.6
1	E	226	GLU	2.6
1	F	52	SER	2.6
2	K	247	TYR	2.5
1	E	141	SER	2.5
2	H	38	ASP	2.5
1	D	65	LEU	2.5
1	A	192	ILE	2.5
1	B	286	ASP	2.5
1	C	128	ASN	2.5
2	J	256	PHE	2.5
2	H	208	ASN	2.5
1	B	77	THR	2.5
1	D	20	GLY	2.5
2	K	62	GLY	2.5
1	A	274	ILE	2.5
1	E	159	VAL	2.5
1	A	21	PHE	2.5
1	A	353	GLN	2.5
1	B	122	ILE	2.5
2	I	359	HIS	2.5

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	76	VAL	2.5
1	A	95	ARG	2.4
2	K	182	ASN	2.4
1	A	217	CYS	2.4
1	F	162	THR	2.4
2	I	71	TYR	2.4
1	E	31	PHE	2.4
1	A	155	SER	2.4
1	C	349	LEU	2.4
1	F	169	TYR	2.4
1	B	139	VAL	2.4
1	D	98	PRO	2.4
1	B	133	TYR	2.4
2	I	140	LEU	2.4
2	K	363	GLN	2.3
1	B	195	GLU	2.3
1	B	253	GLU	2.3
1	A	103	VAL	2.3
2	K	366	PHE	2.3
2	I	180	MET	2.3
1	E	225	GLN	2.3
2	J	160	THR	2.3
1	B	198	TYR	2.3
1	F	180	LEU	2.3
1	F	375	PHE	2.3
2	I	341	GLU	2.3
1	E	160	THR	2.3
1	A	104	LEU	2.3
1	D	309	ILE	2.3
2	K	61	SER	2.3
1	B	109	PRO	2.3
2	J	327	ASN	2.3
2	K	264	THR	2.3
1	B	258	PRO	2.3
1	F	329	ILE	2.3
1	A	167	GLU	2.3
1	F	23	GLY	2.3
1	B	108	ALA	2.3
1	B	374	CYS	2.2
2	K	37	LEU	2.2
2	J	222	PRO	2.2
2	J	49	TYR	2.2

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	257	VAL	2.2
1	B	22	ALA	2.2
1	D	181	ALA	2.2
1	D	180	LEU	2.2
1	E	296	ASN	2.2
1	B	23	GLY	2.2
1	D	129	THR	2.2
2	H	203	ARG	2.2
2	K	254	THR	2.2
1	B	261	LEU	2.2
1	A	180	LEU	2.2
2	H	20	SER	2.2
2	I	141	SER	2.2
1	E	154	ASP	2.2
2	H	163	THR	2.2
1	E	133	TYR	2.2
1	B	213	LYS	2.2
1	B	12	ASN	2.2
1	B	248	ILE	2.2
2	H	209	THR	2.2
1	B	53	TYR	2.2
1	A	200	PHE	2.2
1	B	179	ASP	2.2
1	C	303	THR	2.2
1	A	79	TRP	2.1
1	A	369	ILE	2.1
2	H	214	PRO	2.1
1	E	153	MET	2.1
2	I	322	ILE	2.1
1	C	158	GLY	2.1
1	E	22	ALA	2.1
1	A	152	VAL	2.1
1	A	86	TRP	2.1
1	A	262	PHE	2.1
1	E	135	ALA	2.1
1	C	33	SER	2.1
2	J	44	LEU	2.1
1	B	340	TRP	2.1
1	E	53	TYR	2.1
1	A	259	GLU	2.1
1	A	178	LEU	2.1
1	B	8	LEU	2.1

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	261	LEU	2.1
1	A	93	GLU	2.1
1	A	151	ILE	2.1
2	I	105	VAL	2.1
1	A	158	GLY	2.1
2	J	93	LEU	2.1
1	A	141	SER	2.1
2	K	259	SER	2.1
1	D	336	LYS	2.1
2	I	49	TYR	2.1
1	B	85	ILE	2.1
2	I	43	ILE	2.1
2	K	359	HIS	2.1
1	E	310	ALA	2.1
1	A	154	ASP	2.1
2	J	130	LEU	2.1
1	A	78	ASN	2.1
1	A	134	VAL	2.1
1	C	362	TYR	2.1
1	D	75	ILE	2.1
1	A	161	HIS	2.1
2	K	104	GLU	2.1
2	H	23	LYS	2.0
1	B	104	LEU	2.0
1	C	122	ILE	2.0
2	I	200	ASP	2.0
2	H	189	LEU	2.0
2	I	323	PHE	2.0
1	D	359	LYS	2.0
1	F	267	LEU	2.0
1	A	278	THR	2.0
1	B	116	ARG	2.0
1	C	70	PRO	2.0
1	A	213	LYS	2.0
1	E	247	VAL	2.0
1	F	354	GLN	2.0
2	H	290	GLN	2.0
1	A	140	LEU	2.0
1	C	293	LEU	2.0
2	I	291	ILE	2.0
2	J	290	GLN	2.0
2	H	150	TYR	2.0

For Manuscript Review

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.

For Manuscript Review