



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:10 am GMT

PDB ID : 3EAB
Title : Crystal structure of Spastin MIT in complex with ESCRT III
Authors : Yang, D.; Rimanchi, N.; Renvoise, B.; Lippincott-Schwartz, J.; Blackstone, C.; Hurley, J.H.
Deposited on : 2008-08-25
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

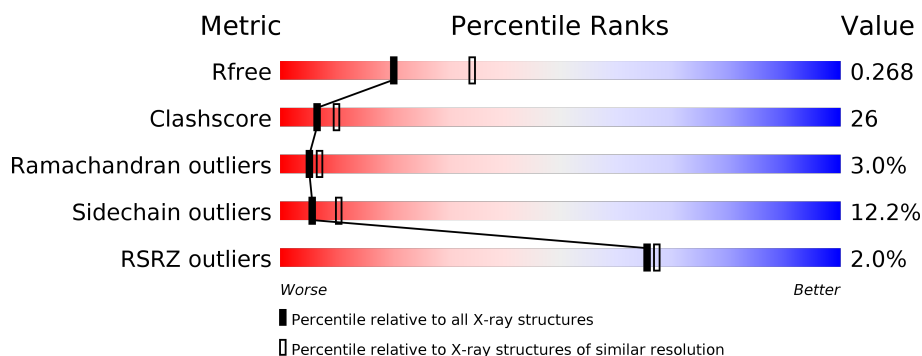
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	89	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>35%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	89	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>7%</div> <div>..</div> </div> </div>
1	C	89	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>37%</div> <div>.</div> </div> </div>
1	D	89	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>33%</div> <div>10%</div> <div>..</div> </div> </div>
1	E	89	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>.</div> </div> </div>
1	F	89	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>37%</div> <div>..</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	50	<div><div></div><div></div><div></div><div></div></div> <div>54%24%•20%</div>
2	H	50	<div><div></div><div></div><div></div><div></div></div> <div>50%14%14%22%</div>
2	I	50	<div><div></div><div></div><div></div><div></div></div> <div>58%14%8%•18%</div>
2	J	50	<div><div></div><div></div><div></div><div></div></div> <div>2%46%18%8%•26%</div>
2	K	50	<div><div></div><div></div><div></div><div></div></div> <div>44%22%8%•24%</div>
2	L	50	<div><div></div><div></div><div></div><div></div></div> <div>40%30%•26%</div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5977 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 Spastin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	0	0
			719	448	129	136	6			
1	B	88	Total	C	N	O	S	0	0	0
			711	443	128	135	5			
1	C	89	Total	C	N	O	S	0	0	0
			719	448	129	136	6			
1	D	88	Total	C	N	O	S	0	0	0
			709	443	128	132	6			
1	E	86	Total	C	N	O	S	0	0	0
			701	438	126	132	5			
1	F	87	Total	C	N	O	S	0	0	0
			701	437	127	131	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	MET	-	EXPRESSION TAG	UNP Q9UBP0
A	109	GLY	-	EXPRESSION TAG	UNP Q9UBP0
A	110	SER	-	EXPRESSION TAG	UNP Q9UBP0
A	111	MET	-	EXPRESSION TAG	UNP Q9UBP0
B	108	MET	-	EXPRESSION TAG	UNP Q9UBP0
B	109	GLY	-	EXPRESSION TAG	UNP Q9UBP0
B	110	SER	-	EXPRESSION TAG	UNP Q9UBP0
B	111	MET	-	EXPRESSION TAG	UNP Q9UBP0
C	108	MET	-	EXPRESSION TAG	UNP Q9UBP0
C	109	GLY	-	EXPRESSION TAG	UNP Q9UBP0
C	110	SER	-	EXPRESSION TAG	UNP Q9UBP0
C	111	MET	-	EXPRESSION TAG	UNP Q9UBP0
D	108	MET	-	EXPRESSION TAG	UNP Q9UBP0
D	109	GLY	-	EXPRESSION TAG	UNP Q9UBP0
D	110	SER	-	EXPRESSION TAG	UNP Q9UBP0
D	111	MET	-	EXPRESSION TAG	UNP Q9UBP0
E	108	MET	-	EXPRESSION TAG	UNP Q9UBP0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	109	GLY	-	EXPRESSION TAG	UNP Q9UBP0
E	110	SER	-	EXPRESSION TAG	UNP Q9UBP0
E	111	MET	-	EXPRESSION TAG	UNP Q9UBP0
F	108	MET	-	EXPRESSION TAG	UNP Q9UBP0
F	109	GLY	-	EXPRESSION TAG	UNP Q9UBP0
F	110	SER	-	EXPRESSION TAG	UNP Q9UBP0
F	111	MET	-	EXPRESSION TAG	UNP Q9UBP0

- Molecule 2 is a protein called CHMP1b.

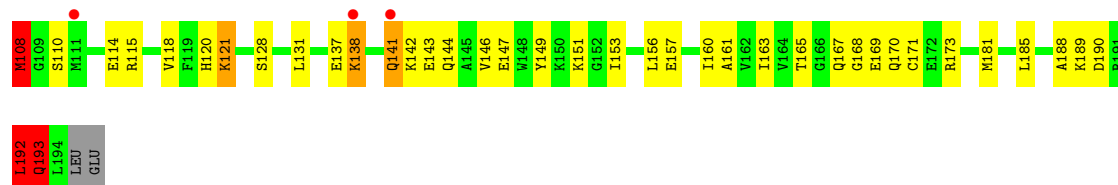
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	40	Total	C	N	O	S	0	0	0
			297	176	53	66	2			
2	H	39	Total	C	N	O	S	0	0	0
			290	170	51	67	2			
2	I	41	Total	C	N	O	S	0	0	0
			307	182	54	69	2			
2	J	37	Total	C	N	O	S	0	0	0
			271	160	47	62	2			
2	K	38	Total	C	N	O	S	0	0	0
			281	167	50	62	2			
2	L	37	Total	C	N	O	S	0	0	0
			271	162	47	60	2			

- Molecule 1: Spastin

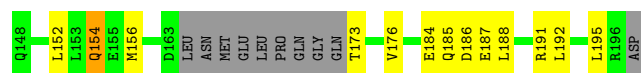




- Molecule 1: Spastin



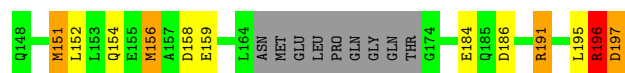
- Molecule 2: CHMP1b



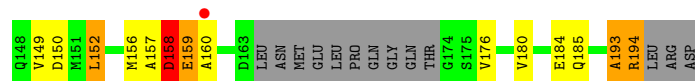
- Molecule 2: CHMP1b



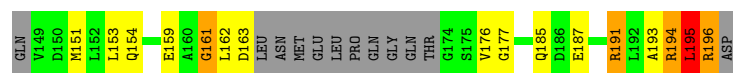
- Molecule 2: CHMP1b



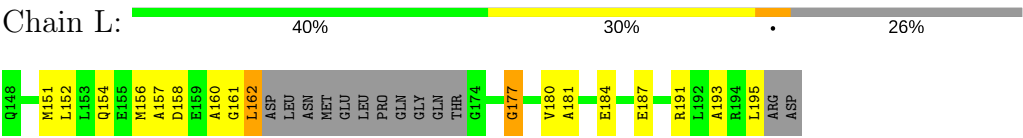
- Molecule 2: CHMP1b



- Molecule 2: CHMP1b



- Molecule 2: CHMP1b



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.97Å 95.49Å 100.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 2.50 47.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (47.65-2.50) 84.6 (47.65-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.29Å)	Xtriage
Refinement program	CNS1.1 and Refmac	Depositor
R, R_{free}	0.232 , 0.268 0.232 , 0.268	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5977	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/725	0.48	0/963
1	B	0.81	3/717 (0.4%)	0.62	1/953 (0.1%)
1	C	0.76	1/725 (0.1%)	0.56	1/963 (0.1%)
1	D	0.47	0/715	0.54	0/951
1	E	0.48	0/707	0.52	0/940
1	F	0.76	2/707 (0.3%)	0.63	1/940 (0.1%)
2	G	0.35	0/295	0.51	0/394
2	H	0.43	0/288	0.56	0/383
2	I	0.36	0/305	0.52	0/406
2	J	0.42	0/269	0.55	0/359
2	K	0.44	0/279	0.60	0/372
2	L	0.34	0/269	0.52	0/359
All	All	0.59	6/6001 (0.1%)	0.56	3/7983 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	E	0	2
1	F	0	1
2	J	0	2
All	All	0	9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	LYS	CE-NZ	15.49	1.87	1.49
1	B	150	LYS	CE-NZ	14.85	1.86	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	121	LYS	CE-NZ	11.64	1.78	1.49
1	F	121	LYS	CD-CE	8.19	1.71	1.51
1	B	121	LYS	CE-NZ	7.81	1.68	1.49
1	B	150	LYS	CD-CE	6.33	1.67	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	121	LYS	CD-CE-NZ	-7.89	93.55	111.70
1	B	150	LYS	CD-CE-NZ	-7.62	94.19	111.70
1	C	150	LYS	CD-CE-NZ	-6.81	96.03	111.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	GLN	Peptide
1	B	138	LYS	Peptide
1	C	138	LYS	Peptide
1	C	166	GLY	Peptide
1	E	166	GLY	Peptide
1	E	191	ARG	Sidechain
1	F	108	MET	Mainchain
2	J	158	ASP	Peptide
2	J	193	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	719	0	733	41	0
1	B	711	0	724	65	1
1	C	719	0	733	27	0
1	D	709	0	727	42	1
1	E	701	0	716	30	0
1	F	701	0	716	46	1
2	G	297	0	288	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	290	0	275	19	0
2	I	307	0	296	15	0
2	J	271	0	257	19	0
2	K	281	0	273	15	0
2	L	271	0	264	23	1
All	All	5977	0	6002	315	3

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 26.

All (315) 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)
1:B:121:LYS:CE	1:B:121:LYS:NZ	1.68	1.51
1:F:121:LYS:NZ	1:F:121:LYS:CE	1.78	1.46
1:B:150:LYS:CE	1:B:150:LYS:NZ	1.86	1.39
1:C:150:LYS:CE	1:C:150:LYS:NZ	1.87	1.37
2:J:194:ARG:N	2:J:194:ARG:HD3	1.12	1.21
2:L:162:LEU:HD23	2:L:162:LEU:N	1.56	1.16
1:D:153:ILE:HD12	1:D:185:LEU:HD12	1.22	1.13
2:L:162:LEU:N	2:L:162:LEU:CD2	2.07	1.12
2:J:194:ARG:N	2:J:194:ARG:CD	2.06	1.12
1:B:167:GLN:HE21	1:E:150:LYS:NZ	1.48	1.11
2:H:196:ARG:HH11	2:H:196:ARG:HG2	1.13	1.10
2:J:193:ALA:C	2:J:194:ARG:HD3	1.70	1.10
2:I:191:ARG:HG3	2:I:191:ARG:HH11	1.05	1.09
1:A:141:GLN:CD	1:A:141:GLN:H	1.55	1.09
1:D:194:LEU:HD13	1:D:194:LEU:O	1.52	1.08
1:F:193:GLN:N	1:F:193:GLN:OE1	1.88	1.05
1:D:193:GLN:O	1:D:195:LEU:N	1.90	1.03
2:K:195:LEU:HD12	2:K:195:LEU:O	1.61	1.00
2:J:159:GLU:N	2:J:159:GLU:OE1	1.93	0.99
1:B:141:GLN:CD	1:B:141:GLN:H	1.61	0.98
1:E:115:ARG:O	1:E:118:VAL:HG22	1.65	0.97
1:A:149:TYR:O	1:A:153:ILE:HD13	1.65	0.97
2:J:194:ARG:HD3	2:J:194:ARG:H	1.23	0.96
2:L:161:GLY:C	2:L:162:LEU:HD22	1.85	0.96
1:C:108:MET:SD	1:C:108:MET:C	2.43	0.96
1:B:153:ILE:HD11	1:B:188:ALA:HB3	1.46	0.95
1:D:195:LEU:C	1:D:195:LEU:HD23	1.86	0.95
2:L:162:LEU:HD23	2:L:162:LEU:H	1.26	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLN:OE1	1:B:141:GLN:N	2.03	0.92
1:F:153:ILE:HD11	1:F:188:ALA:HB3	1.51	0.91
1:C:138:LYS:HB2	1:C:141:GLN:OE1	1.72	0.89
2:H:196:ARG:HG2	2:H:196:ARG:NH1	1.85	0.88
1:B:153:ILE:HD12	1:B:185:LEU:HD12	1.54	0.88
2:J:158:ASP:C	2:J:159:GLU:OE1	2.13	0.87
1:F:108:MET:HG2	1:F:108:MET:O	1.74	0.87
1:D:147:GLU:OE1	1:D:151:LYS:NZ	2.06	0.86
1:F:193:GLN:CA	1:F:193:GLN:OE1	2.24	0.86
1:B:131:LEU:HD21	2:H:192:LEU:HD13	1.58	0.86
1:B:150:LYS:HZ3	1:F:167:GLN:HE21	1.17	0.86
2:I:191:ARG:NH1	2:I:191:ARG:HG3	1.82	0.86
1:A:137:GLU:OE2	1:A:137:GLU:HA	1.75	0.86
2:H:150:ASP:N	2:H:150:ASP:OD1	2.07	0.84
1:F:141:GLN:CD	1:F:141:GLN:H	1.81	0.84
1:B:141:GLN:CD	1:B:141:GLN:N	2.30	0.84
1:B:167:GLN:HE21	1:E:150:LYS:HZ2	1.20	0.84
2:I:195:LEU:O	2:I:197:ASP:N	2.11	0.83
1:E:138:LYS:O	1:E:142:LYS:HE2	1.79	0.82
1:B:167:GLN:HE21	1:E:150:LYS:HZ3	1.26	0.82
2:H:196:ARG:O	2:H:196:ARG:CG	2.28	0.82
1:D:125:GLU:OE1	1:D:125:GLU:HA	1.79	0.82
2:L:161:GLY:C	2:L:162:LEU:CD2	2.44	0.82
1:B:141:GLN:HA	1:B:143:GLU:OE2	1.79	0.81
2:G:156:MET:CE	2:L:156:MET:HG2	2.10	0.81
1:A:115:ARG:O	1:A:118:VAL:HG22	1.80	0.80
1:A:141:GLN:CD	1:A:141:GLN:N	2.31	0.80
1:B:150:LYS:HZ3	1:F:167:GLN:NE2	1.80	0.80
1:B:150:LYS:HZ3	1:F:167:GLN:CG	1.94	0.80
2:I:196:ARG:HH11	2:I:196:ARG:HG3	1.45	0.79
1:D:141:GLN:H	1:D:141:GLN:CD	1.84	0.79
1:A:108:MET:O	1:A:110:SER:N	2.14	0.79
1:B:115:ARG:O	1:B:118:VAL:HG22	1.82	0.79
1:A:137:GLU:CA	1:A:137:GLU:OE2	2.31	0.78
1:E:141:GLN:N	1:E:141:GLN:OE1	2.16	0.78
1:F:153:ILE:HD11	1:F:188:ALA:CB	2.14	0.78
1:D:153:ILE:HD11	1:D:188:ALA:HB3	1.66	0.77
1:D:194:LEU:HD13	1:D:194:LEU:C	2.04	0.77
1:A:167:GLN:HA	1:A:167:GLN:OE1	1.83	0.76
1:B:150:LYS:NZ	1:F:167:GLN:HE21	1.83	0.76
2:K:195:LEU:O	2:K:195:LEU:CD1	2.34	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD13	2:G:191:ARG:HG2	1.67	0.75
1:F:167:GLN:HA	1:F:167:GLN:OE1	1.86	0.75
1:B:167:GLN:NE2	1:E:150:LYS:NZ	2.29	0.75
2:K:195:LEU:HD12	2:K:195:LEU:C	2.06	0.74
1:D:141:GLN:CD	1:D:141:GLN:N	2.41	0.74
1:D:195:LEU:O	1:D:195:LEU:HD23	1.87	0.73
1:A:141:GLN:NE2	1:A:141:GLN:H	1.87	0.73
1:F:138:LYS:O	1:F:142:LYS:HE2	1.88	0.73
2:J:193:ALA:C	2:J:194:ARG:CD	2.50	0.73
1:A:153:ILE:HD11	1:A:188:ALA:HB1	1.69	0.73
2:I:195:LEU:C	2:I:197:ASP:H	1.92	0.72
1:B:167:GLN:HG2	1:E:150:LYS:NZ	2.05	0.72
1:B:150:LYS:HZ3	1:F:167:GLN:HG2	1.54	0.72
1:B:125:GLU:OE1	1:B:125:GLU:HA	1.90	0.72
1:D:120:HIS:HB2	1:D:181:MET:CE	2.20	0.72
1:D:153:ILE:HD12	1:D:185:LEU:CD1	2.12	0.71
1:D:141:GLN:OE1	1:D:141:GLN:N	2.22	0.71
1:A:127:ILE:HD11	1:A:152:GLY:HA3	1.72	0.71
1:D:115:ARG:O	1:D:118:VAL:HG22	1.91	0.70
2:L:160:ALA:HB3	2:L:162:LEU:HD21	1.73	0.70
2:K:161:GLY:O	2:K:162:LEU:HG	1.92	0.70
1:F:121:LYS:NZ	1:F:121:LYS:CD	2.54	0.70
1:D:137:GLU:OE1	1:D:137:GLU:HA	1.92	0.69
2:G:156:MET:HE1	2:L:156:MET:HG2	1.72	0.69
1:D:160:ILE:HD11	1:D:181:MET:HB2	1.75	0.69
1:F:153:ILE:CD1	1:F:188:ALA:HB3	2.22	0.69
1:B:150:LYS:NZ	1:F:167:GLN:CG	2.55	0.68
1:B:159:GLY:HA3	1:B:181:MET:HE1	1.76	0.68
1:C:115:ARG:O	1:C:118:VAL:HG22	1.92	0.68
2:G:187:GLU:HG3	2:L:152:LEU:HG	1.75	0.68
1:B:150:LYS:NZ	1:F:167:GLN:HG2	2.08	0.68
1:C:108:MET:SD	1:C:109:GLY:N	2.67	0.68
2:G:156:MET:HE3	2:L:156:MET:HG2	1.76	0.67
1:F:114:GLU:O	1:F:118:VAL:HG13	1.94	0.67
1:C:160:ILE:HD11	1:C:181:MET:HB2	1.75	0.67
1:D:168:GLY:O	1:D:172:GLU:HG3	1.95	0.67
1:B:131:LEU:HD13	2:H:191:ARG:HD3	1.76	0.67
1:B:150:LYS:HE3	1:B:196:GLU:OE2	1.95	0.66
1:F:108:MET:CG	1:F:108:MET:O	2.41	0.66
1:B:150:LYS:NZ	1:B:150:LYS:CD	2.58	0.66
1:B:121:LYS:CD	1:B:121:LYS:NZ	2.56	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ASN:OD1	2:J:185:GLN:NE2	2.29	0.65
2:K:193:ALA:O	2:K:196:ARG:HG3	1.95	0.65
2:G:154:GLN:NE2	2:G:154:GLN:HA	2.12	0.65
1:C:150:LYS:NZ	1:C:150:LYS:CD	2.60	0.65
1:A:127:ILE:CD1	1:A:152:GLY:HA3	2.27	0.64
1:F:120:HIS:HB2	1:F:181:MET:CE	2.27	0.64
1:E:138:LYS:HB2	1:E:141:GLN:NE2	2.13	0.64
1:D:120:HIS:HB2	1:D:181:MET:HE2	1.79	0.63
2:I:195:LEU:C	2:I:197:ASP:N	2.51	0.63
2:J:156:MET:O	2:J:159:GLU:HG2	1.98	0.63
1:A:174:ALA:O	1:A:177:LEU:HB3	1.99	0.63
2:K:194:ARG:O	2:K:194:ARG:HG3	1.97	0.63
1:C:168:GLY:O	1:C:172:GLU:HG3	1.98	0.62
1:D:195:LEU:C	1:D:195:LEU:CD2	2.61	0.62
1:D:118:VAL:HG23	1:D:119:PHE:N	2.15	0.62
1:D:194:LEU:CD1	1:D:194:LEU:C	2.67	0.62
1:A:131:LEU:O	1:A:135:GLU:OE1	2.18	0.62
2:J:157:ALA:O	2:J:159:GLU:N	2.33	0.62
1:F:141:GLN:CD	1:F:141:GLN:N	2.53	0.62
1:B:167:GLN:NE2	1:E:150:LYS:HZ3	1.92	0.61
2:H:196:ARG:O	2:H:196:ARG:HG2	1.97	0.61
1:A:115:ARG:O	1:A:118:VAL:CG2	2.48	0.61
2:I:196:ARG:NH1	2:I:196:ARG:HG3	2.14	0.61
1:F:193:GLN:HA	1:F:193:GLN:OE1	1.99	0.61
1:B:137:GLU:OE2	1:B:137:GLU:HA	2.00	0.60
1:B:180:LYS:HE3	2:H:182:SER:OG	2.01	0.60
2:H:196:ARG:CG	2:H:196:ARG:NH1	2.62	0.60
1:B:153:ILE:HD11	1:B:188:ALA:CB	2.25	0.60
2:L:177:GLY:O	2:L:180:VAL:HG22	2.02	0.60
1:C:114:GLU:OE2	1:C:117:ARG:NH2	2.31	0.60
2:K:194:ARG:C	2:K:196:ARG:H	2.05	0.60
1:A:137:GLU:HG3	1:A:141:GLN:O	2.02	0.60
1:E:115:ARG:O	1:E:118:VAL:CG2	2.46	0.60
1:B:167:GLN:CG	1:E:150:LYS:HZ3	2.15	0.59
2:H:196:ARG:HG3	2:H:196:ARG:O	2.01	0.59
1:D:131:LEU:O	1:D:135:GLU:HG3	2.03	0.59
1:E:138:LYS:HB2	1:E:141:GLN:CD	2.23	0.59
1:B:131:LEU:HD21	2:H:192:LEU:CD1	2.31	0.58
1:C:147:GLU:OE1	1:C:151:LYS:NZ	2.24	0.58
1:D:160:ILE:CD1	1:D:181:MET:HB2	2.32	0.58
1:A:168:GLY:O	1:A:171:CYS:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ILE:HD11	1:C:181:MET:CB	2.33	0.58
2:H:195:LEU:O	2:H:197:ASP:N	2.33	0.58
2:G:156:MET:HE3	2:L:156:MET:CG	2.35	0.57
2:H:160:ALA:HB3	2:H:162:LEU:HD12	1.85	0.57
1:B:167:GLN:HG2	1:E:150:LYS:HZ1	1.68	0.57
1:D:112:GLU:HG2	1:D:163:ILE:O	2.05	0.57
1:A:180:LYS:NZ	2:G:186:ASP:OD1	2.32	0.56
1:A:167:GLN:OE1	1:A:167:GLN:CA	2.54	0.56
1:B:192:LEU:CD2	1:B:196:GLU:HB2	2.36	0.56
1:A:184:ASN:OD1	2:G:185:GLN:NE2	2.39	0.56
1:D:193:GLN:O	1:D:194:LEU:C	2.43	0.56
1:E:137:GLU:HA	1:E:137:GLU:OE2	2.06	0.56
1:F:153:ILE:HG23	1:F:185:LEU:CD1	2.35	0.56
2:L:160:ALA:CB	2:L:162:LEU:HD21	2.35	0.56
1:A:156:LEU:O	1:A:160:ILE:HG12	2.06	0.55
1:D:118:VAL:CG2	1:D:119:PHE:N	2.70	0.55
1:F:137:GLU:OE1	1:F:144:GLN:OE1	2.25	0.55
1:F:120:HIS:HB2	1:F:181:MET:HE2	1.87	0.55
1:F:115:ARG:O	1:F:118:VAL:HG22	2.07	0.55
1:B:167:GLN:HG2	1:E:150:LYS:HZ3	1.72	0.55
1:F:168:GLY:O	1:F:171:CYS:HB2	2.06	0.55
2:G:154:GLN:CA	2:G:154:GLN:HE21	2.19	0.54
2:L:157:ALA:O	2:L:162:LEU:HD23	2.08	0.54
1:E:141:GLN:N	1:E:141:GLN:CD	2.59	0.54
1:B:192:LEU:HD22	1:B:196:GLU:HB2	1.89	0.54
1:F:131:LEU:HD13	2:L:191:ARG:HD3	1.90	0.54
2:H:176:VAL:HG13	2:H:177:GLY:N	2.23	0.54
1:E:141:GLN:H	1:E:141:GLN:CD	2.11	0.54
1:B:141:GLN:CA	1:B:143:GLU:OE2	2.54	0.54
1:D:109:GLY:HA2	1:D:112:GLU:OE2	2.08	0.54
1:C:160:ILE:CD1	1:C:181:MET:HB2	2.39	0.53
1:E:153:ILE:HG23	1:E:185:LEU:HD11	1.89	0.53
1:A:137:GLU:OE2	1:A:137:GLU:N	2.41	0.53
2:J:158:ASP:OD2	2:J:184:GLU:OE1	2.26	0.53
1:F:143:GLU:HA	1:F:146:VAL:HG23	1.90	0.53
2:K:187:GLU:OE2	2:K:191:ARG:HD2	2.08	0.52
1:F:156:LEU:O	1:F:160:ILE:HG13	2.10	0.52
1:F:193:GLN:N	1:F:193:GLN:CD	2.62	0.52
2:J:157:ALA:C	2:J:159:GLU:N	2.62	0.52
1:E:184:ASN:OD1	2:K:185:GLN:NE2	2.43	0.51
1:B:174:ALA:O	1:B:177:LEU:HB3	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLN:HB3	1:C:155:GLU:HG3	1.93	0.51
2:H:196:ARG:HH11	2:H:196:ARG:CG	1.99	0.51
1:C:174:ALA:O	1:C:177:LEU:HB3	2.11	0.51
2:K:195:LEU:CD1	2:K:195:LEU:C	2.79	0.51
1:E:111:MET:HG3	1:E:111:MET:O	1.98	0.51
1:F:161:ALA:O	1:F:163:ILE:HD12	2.10	0.51
1:D:154:GLU:O	1:D:158:LYS:HG3	2.11	0.50
1:E:138:LYS:HB2	1:E:141:GLN:OE1	2.11	0.50
1:A:153:ILE:HG23	1:A:185:LEU:CD1	2.41	0.50
1:C:160:ILE:CD1	1:C:178:GLN:O	2.59	0.50
2:G:156:MET:CE	2:L:156:MET:CG	2.85	0.50
2:G:152:LEU:HG	2:L:187:GLU:HG3	1.94	0.50
1:A:169:GLU:O	1:A:173:ARG:HG3	2.11	0.50
2:L:158:ASP:OD2	2:L:184:GLU:OE2	2.30	0.50
1:F:192:LEU:C	1:F:193:GLN:OE1	2.49	0.50
2:J:157:ALA:C	2:J:159:GLU:H	2.15	0.50
2:H:176:VAL:HG13	2:H:177:GLY:H	1.77	0.49
2:L:161:GLY:O	2:L:162:LEU:HD22	2.12	0.49
1:F:147:GLU:OE1	1:F:151:LYS:HE3	2.12	0.49
2:K:176:VAL:HG13	2:K:177:GLY:N	2.28	0.49
1:A:153:ILE:HG23	1:A:185:LEU:HD11	1.95	0.49
1:B:153:ILE:CD1	1:B:185:LEU:HD12	2.35	0.49
1:D:141:GLN:HA	1:D:143:GLU:OE2	2.12	0.49
2:L:162:LEU:HD22	2:L:162:LEU:N	2.00	0.48
1:C:138:LYS:O	1:C:142:LYS:HE2	2.13	0.48
2:G:192:LEU:O	2:G:195:LEU:HB2	2.13	0.48
1:C:153:ILE:O	1:C:157:GLU:HG3	2.13	0.48
1:A:137:GLU:OE1	1:A:144:GLN:NE2	2.47	0.48
1:F:146:VAL:HG13	1:F:192:LEU:HD21	1.95	0.48
2:L:154:GLN:HA	2:L:154:GLN:OE1	2.13	0.48
2:G:154:GLN:NE2	2:G:154:GLN:CA	2.72	0.48
1:D:160:ILE:HD11	1:D:181:MET:CB	2.43	0.48
1:E:118:VAL:HG23	1:E:119:PHE:N	2.28	0.48
2:I:158:ASP:OD1	2:I:184:GLU:OE1	2.30	0.48
2:K:162:LEU:O	2:K:163:ASP:HB3	2.14	0.48
1:B:127:ILE:HG22	1:B:127:ILE:O	2.13	0.48
1:B:192:LEU:C	1:B:194:LEU:H	2.17	0.48
1:C:114:GLU:HA	1:C:114:GLU:OE2	2.13	0.48
2:H:173:THR:O	2:H:174:GLY:C	2.51	0.48
2:L:180:VAL:HG23	2:L:181:ALA:N	2.28	0.48
1:C:138:LYS:HA	1:C:138:LYS:HD2	1.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:LEU:C	2:H:197:ASP:H	2.17	0.47
1:F:108:MET:C	1:F:108:MET:SD	2.92	0.47
1:A:108:MET:C	1:A:110:SER:N	2.68	0.47
1:D:193:GLN:C	1:D:195:LEU:H	2.17	0.47
1:B:192:LEU:HD22	1:B:196:GLU:CB	2.45	0.47
1:D:167:GLN:O	1:D:167:GLN:HG3	2.15	0.47
1:D:193:GLN:C	1:D:195:LEU:N	2.63	0.47
2:I:156:MET:HA	2:I:156:MET:CE	2.44	0.47
1:B:127:ILE:CD1	1:B:152:GLY:HA3	2.45	0.47
1:F:138:LYS:HA	1:F:138:LYS:HD3	1.77	0.46
1:B:138:LYS:HA	1:B:138:LYS:HD3	1.42	0.46
1:A:163:ILE:CD1	1:B:163:ILE:HD11	2.45	0.46
2:I:196:ARG:O	2:I:197:ASP:C	2.53	0.46
2:K:194:ARG:C	2:K:196:ARG:N	2.68	0.46
1:A:182:MET:HG2	1:B:182:MET:HG3	1.98	0.46
1:B:138:LYS:HB2	1:B:141:GLN:CD	2.37	0.46
2:H:188:LEU:HD12	2:H:188:LEU:HA	1.70	0.46
2:I:156:MET:O	2:I:159:GLU:HB3	2.15	0.46
1:B:109:GLY:N	1:B:112:GLU:HG3	2.32	0.45
1:C:167:GLN:OE1	1:C:167:GLN:HA	2.16	0.45
2:J:194:ARG:CG	2:J:194:ARG:HH11	2.29	0.45
2:K:151:MET:O	2:K:154:GLN:HB3	2.17	0.45
1:D:125:GLU:OE1	1:D:125:GLU:CA	2.57	0.45
1:B:153:ILE:HD12	1:B:185:LEU:CD1	2.35	0.45
1:D:156:LEU:O	1:D:160:ILE:HG12	2.17	0.45
1:E:153:ILE:HG23	1:E:185:LEU:CD1	2.47	0.45
1:A:182:MET:HG3	1:B:182:MET:SD	2.57	0.45
1:E:174:ALA:O	1:E:177:LEU:HB3	2.17	0.45
1:C:137:GLU:HA	1:C:137:GLU:OE2	2.17	0.45
1:B:153:ILE:HG23	1:B:185:LEU:HD11	1.99	0.44
1:A:133:ILE:O	1:A:134:ASP:C	2.54	0.44
1:D:138:LYS:HB2	1:D:141:GLN:OE1	2.17	0.44
1:A:111:MET:O	1:A:115:ARG:HG3	2.17	0.44
1:A:182:MET:CG	1:B:182:MET:SD	3.05	0.44
1:D:139:ALA:HA	1:D:142:LYS:HE2	1.99	0.44
2:J:194:ARG:NH1	2:J:194:ARG:HG2	2.33	0.44
1:A:170:GLN:O	1:A:173:ARG:HB2	2.18	0.44
1:B:169:GLU:O	1:B:173:ARG:HG3	2.18	0.44
1:F:137:GLU:O	1:F:138:LYS:O	2.36	0.43
1:F:157:GLU:HA	1:F:160:ILE:HD12	1.99	0.43
1:B:138:LYS:HB3	1:B:139:ALA:H	1.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD21	2:G:192:LEU:HD23	2.01	0.43
1:B:153:ILE:HG23	1:B:185:LEU:CD1	2.49	0.43
1:B:192:LEU:C	1:B:194:LEU:N	2.70	0.43
2:K:161:GLY:C	2:K:162:LEU:HG	2.39	0.43
2:J:152:LEU:HA	2:J:152:LEU:HD12	1.82	0.43
1:C:180:LYS:HE2	2:I:186:ASP:OD1	2.18	0.43
1:C:118:VAL:HG23	1:C:119:PHE:N	2.32	0.42
1:C:160:ILE:HD11	1:C:182:MET:N	2.34	0.42
2:I:151:MET:HG2	2:I:152:LEU:HD13	2.00	0.42
1:F:185:LEU:HD11	1:F:189:LYS:HE3	2.00	0.42
1:A:118:VAL:HG23	1:A:119:PHE:N	2.35	0.42
2:I:151:MET:HB3	2:I:151:MET:HE3	1.83	0.42
1:A:160:ILE:CD1	1:A:181:MET:HB2	2.49	0.42
1:D:138:LYS:O	1:D:142:LYS:HG3	2.19	0.42
1:E:125:GLU:C	1:E:125:GLU:OE1	2.58	0.42
1:C:176:ARG:O	1:C:180:LYS:HG3	2.20	0.42
1:F:153:ILE:HG23	1:F:185:LEU:HD11	2.02	0.42
2:J:159:GLU:HB2	2:J:160:ALA:H	1.64	0.42
1:D:188:ALA:O	1:D:191:ARG:N	2.51	0.42
1:C:133:ILE:O	1:C:134:ASP:C	2.58	0.42
1:B:127:ILE:HD11	1:B:152:GLY:HA3	2.02	0.41
1:E:168:GLY:O	1:E:171:CYS:HB2	2.20	0.41
2:I:191:ARG:CG	2:I:191:ARG:HH11	1.94	0.41
1:B:137:GLU:O	1:B:138:LYS:O	2.38	0.41
1:B:150:LYS:HZ3	1:F:167:GLN:CD	2.24	0.41
2:L:193:ALA:C	2:L:195:LEU:H	2.21	0.41
1:B:168:GLY:HA2	1:E:196:GLU:OE1	2.21	0.41
1:E:114:GLU:HA	1:E:114:GLU:OE1	2.20	0.41
2:J:150:ASP:OD2	2:J:152:LEU:HB2	2.21	0.41
1:F:149:TYR:O	1:F:153:ILE:HG12	2.20	0.41
1:A:153:ILE:HD11	1:A:188:ALA:CB	2.44	0.41
1:F:169:GLU:O	1:F:173:ARG:HG3	2.20	0.41
2:J:176:VAL:O	2:J:180:VAL:HG23	2.21	0.41
1:A:163:ILE:HD12	1:B:163:ILE:HD11	2.03	0.40
1:E:141:GLN:HA	1:E:143:GLU:OE2	2.21	0.40
2:G:195:LEU:HA	2:G:195:LEU:HD23	1.75	0.40
1:B:133:ILE:O	1:B:134:ASP:C	2.57	0.40
1:C:118:VAL:CG2	1:C:119:PHE:N	2.84	0.40
1:A:124:PHE:CZ	2:G:184:GLU:HG2	2.57	0.40
1:B:150:LYS:NZ	1:F:167:GLN:HG3	2.34	0.40
1:D:175:ARG:HA	1:D:178:GLN:HE21	1.87	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:156:MET:CE	2:L:156:MET:CE[2_555]	1.72	0.48
1:B:147:GLU:OE2	1:D:144:GLN:NE2[4_457]	1.89	0.31
1:F:144:GLN:NE2	1:F:147:GLU:OE2[2_555]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	87/89 (98%)	78 (90%)	6 (7%)	3 (3%)	4	5
1	B	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	15	27
1	C	87/89 (98%)	85 (98%)	0	2 (2%)	7	11
1	D	86/89 (97%)	76 (88%)	6 (7%)	4 (5%)	3	3
1	E	84/89 (94%)	82 (98%)	1 (1%)	1 (1%)	15	27
1	F	85/89 (96%)	79 (93%)	3 (4%)	3 (4%)	4	5
2	G	36/50 (72%)	33 (92%)	3 (8%)	0	100	100
2	H	35/50 (70%)	30 (86%)	3 (9%)	2 (6%)	2	2
2	I	37/50 (74%)	33 (89%)	3 (8%)	1 (3%)	6	9
2	J	33/50 (66%)	30 (91%)	2 (6%)	1 (3%)	5	7
2	K	34/50 (68%)	29 (85%)	3 (9%)	2 (6%)	2	1
2	L	33/50 (66%)	29 (88%)	2 (6%)	2 (6%)	2	1
All	All	723/834 (87%)	665 (92%)	36 (5%)	22 (3%)	5	7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLY
1	A	138	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	138	LYS
1	C	138	LYS
1	D	193	GLN
1	D	194	LEU
1	E	138	LYS
1	F	138	LYS
2	H	174	GLY
2	I	196	ARG
1	A	137	GLU
1	C	109	GLY
1	D	138	LYS
1	D	168	GLY
1	F	193	GLN
2	H	196	ARG
2	J	158	ASP
2	K	161	GLY
2	K	195	LEU
1	F	192	LEU
2	L	151	MET
2	L	177	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	74/74 (100%)	62 (84%)	12 (16%)	3	5
1	B	73/74 (99%)	64 (88%)	9 (12%)	5	10
1	C	74/74 (100%)	67 (90%)	7 (10%)	10	19
1	D	73/74 (99%)	64 (88%)	9 (12%)	5	10
1	E	72/74 (97%)	68 (94%)	4 (6%)	25	45
1	F	72/74 (97%)	63 (88%)	9 (12%)	5	10
2	G	32/41 (78%)	28 (88%)	4 (12%)	5	10
2	H	31/41 (76%)	26 (84%)	5 (16%)	3	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	33/41 (80%)	27 (82%)	6 (18%)	2	3
2	J	29/41 (71%)	25 (86%)	4 (14%)	4	8
2	K	30/41 (73%)	24 (80%)	6 (20%)	1	2
2	L	29/41 (71%)	28 (97%)	1 (3%)	42	69
All	All	622/690 (90%)	546 (88%)	76 (12%)	6	10

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	MET
1	A	111	MET
1	A	135	GLU
1	A	137	GLU
1	A	138	LYS
1	A	141	GLN
1	A	143	GLU
1	A	153	ILE
1	A	165	THR
1	A	167	GLN
1	A	170	GLN
1	A	192	LEU
1	B	110	SER
1	B	111	MET
1	B	121	LYS
1	B	125	GLU
1	B	138	LYS
1	B	141	GLN
1	B	147	GLU
1	B	192	LEU
1	B	194	LEU
1	C	108	MET
1	C	110	SER
1	C	111	MET
1	C	132	ARG
1	C	138	LYS
1	C	143	GLU
1	C	192	LEU
1	D	112	GLU
1	D	141	GLN
1	D	144	GLN
1	D	153	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	165	THR
1	D	167	GLN
1	D	190	ASP
1	D	194	LEU
1	D	195	LEU
1	E	111	MET
1	E	125	GLU
1	E	141	GLN
1	E	192	LEU
1	F	108	MET
1	F	110	SER
1	F	128	SER
1	F	141	GLN
1	F	165	THR
1	F	170	GLN
1	F	190	ASP
1	F	192	LEU
1	F	193	GLN
2	G	154	GLN
2	G	173	THR
2	G	176	VAL
2	G	188	LEU
2	H	150	ASP
2	H	173	THR
2	H	188	LEU
2	H	192	LEU
2	H	195	LEU
2	I	151	MET
2	I	154	GLN
2	I	156	MET
2	I	191	ARG
2	I	196	ARG
2	I	197	ASP
2	J	149	VAL
2	J	152	LEU
2	J	159	GLU
2	J	194	ARG
2	K	153	LEU
2	K	159	GLU
2	K	191	ARG
2	K	194	ARG
2	K	195	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	196	ARG
2	L	162	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	178	GLN
1	A	184	ASN
1	B	144	GLN
1	B	167	GLN
1	B	178	GLN
1	B	184	ASN
1	C	178	GLN
1	C	184	ASN
1	D	144	GLN
1	D	178	GLN
1	D	184	ASN
1	E	178	GLN
1	E	184	ASN
1	F	144	GLN
1	F	167	GLN
1	F	178	GLN
1	F	184	ASN
2	G	154	GLN
2	G	185	GLN
2	H	185	GLN
2	I	185	GLN
2	J	154	GLN
2	J	185	GLN
2	K	185	GLN
2	L	185	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 [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.

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, 95th 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	89/89 (100%)	-0.23	3 (3%) 46 48	30, 53, 106, 120	0
1	B	88/89 (98%)	-0.46	1 (1%) 80 81	29, 46, 92, 121	0
1	C	89/89 (100%)	-0.44	3 (3%) 46 48	25, 44, 82, 119	0
1	D	88/89 (98%)	-0.18	2 (2%) 61 63	34, 55, 92, 110	0
1	E	86/89 (96%)	-0.47	2 (2%) 61 63	28, 47, 93, 124	0
1	F	87/89 (97%)	-0.33	3 (3%) 46 48	37, 54, 85, 126	0
2	G	40/50 (80%)	-0.42	0 100 100	37, 50, 81, 95	0
2	H	39/50 (78%)	-0.54	0 100 100	28, 46, 88, 97	0
2	I	41/50 (82%)	-0.46	0 100 100	26, 45, 84, 94	0
2	J	37/50 (74%)	-0.07	1 (2%) 55 58	34, 45, 89, 95	0
2	K	38/50 (76%)	-0.18	0 100 100	29, 43, 85, 98	0
2	L	37/50 (74%)	-0.55	0 100 100	34, 47, 69, 79	0
All	All	759/834 (91%)	-0.36	15 (1%) 65 67	25, 49, 92, 126	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	MET	4.0
1	F	138	LYS	3.4
1	A	108	MET	3.3
1	A	167	GLN	2.9
1	E	138	LYS	2.7
1	D	163	ILE	2.7
1	C	138	LYS	2.7
2	J	160	ALA	2.6
1	D	111	MET	2.6
1	C	111	MET	2.6
1	F	141	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	111	MET	2.4
1	E	165	THR	2.4
1	C	141	GLN	2.2
1	B	138	LYS	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.