Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2022 – 04:10 pm BST

PDB ID	:	7ZYH
Title	:	Crystal structure of human CPSF30 in complex with hFip1
Authors	:	Muckenfuss, L.M.; Jinek, M.; Migenda Herranz, A.C.; Clerici, M.
Deposited on	:	2022-05-24
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

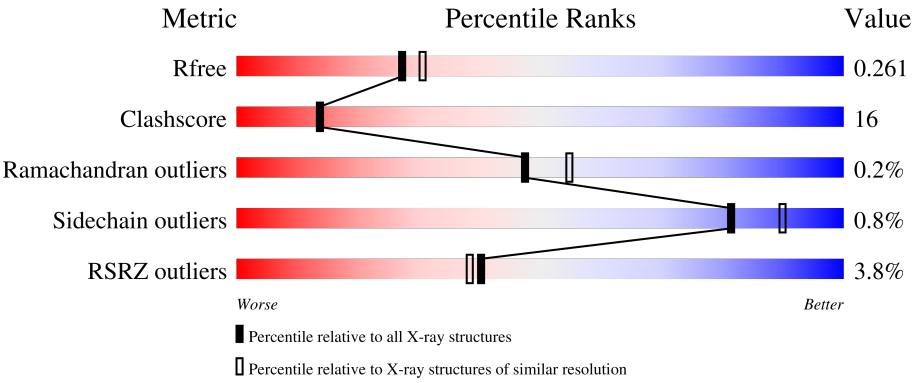
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	64	62% 14% 23%
1	D	64	2% 52% 23% 25%
1	G	64	2% 58% 19% 23%
1	J	64	3% 44% 31% 25%
2	B	69	3% 43% 12% 45%

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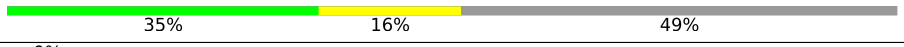
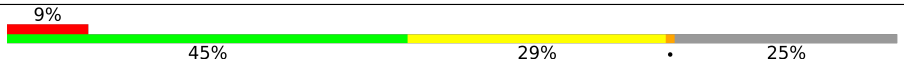
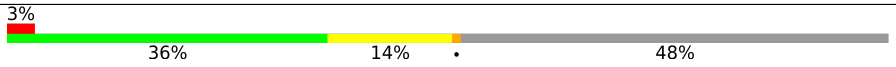
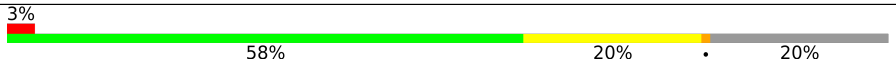
Mol	Chain	Length	Quality of chain
2	C	69	
2	E	69	
2	F	69	
2	H	69	
2	I	69	
2	K	69	
2	L	69	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9075 atoms, of which 4344 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 Cleavage and polyadenylation specificity factor subunit 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	49	Total	C	H	N	O	S	0	0	0
			796	261	386	80	62	7			
1	D	48	Total	C	H	N	O	S	0	0	0
			774	255	373	78	61	7			
1	G	49	Total	C	H	N	O	S	0	0	0
			800	262	391	80	60	7			
1	J	48	Total	C	H	N	O	S	0	0	0
			774	255	373	78	61	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	-	expression tag	UNP O95639
A	116	ASN	-	expression tag	UNP O95639
A	117	ALA	-	expression tag	UNP O95639
D	115	SER	-	expression tag	UNP O95639
D	116	ASN	-	expression tag	UNP O95639
D	117	ALA	-	expression tag	UNP O95639
G	115	SER	-	expression tag	UNP O95639
G	116	ASN	-	expression tag	UNP O95639
G	117	ALA	-	expression tag	UNP O95639
J	115	SER	-	expression tag	UNP O95639
J	116	ASN	-	expression tag	UNP O95639
J	117	ALA	-	expression tag	UNP O95639

- Molecule 2 is a protein called Isoform 4 of Pre-mRNA 3'-end-processing factor FIP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	38	Total	C	H	N	O	S	0	0	0
			634	209	308	57	58	2			
2	C	53	Total	C	H	N	O	S	0	0	0
			847	279	410	73	84	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	35	Total	C	H	N	O	S	0	0	0
			596	197	290	54	53	2			
2	F	52	Total	C	H	N	O	S	0	0	0
			823	273	397	69	83	1			
2	H	36	Total	C	H	N	O	S	0	0	0
			603	199	293	55	54	2			
2	I	55	Total	C	H	N	O	S	0	0	0
			878	288	425	76	87	2			
2	K	35	Total	C	H	N	O	S	0	0	0
			596	197	290	54	53	2			
2	L	54	Total	C	H	N	O	S	0	0	0
			848	280	408	72	87	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	127	SER	-	expression tag	UNP Q6UN15-4
B	128	ASN	-	expression tag	UNP Q6UN15-4
B	129	ALA	-	expression tag	UNP Q6UN15-4
C	127	SER	-	expression tag	UNP Q6UN15-4
C	128	ASN	-	expression tag	UNP Q6UN15-4
C	129	ALA	-	expression tag	UNP Q6UN15-4
E	127	SER	-	expression tag	UNP Q6UN15-4
E	128	ASN	-	expression tag	UNP Q6UN15-4
E	129	ALA	-	expression tag	UNP Q6UN15-4
F	127	SER	-	expression tag	UNP Q6UN15-4
F	128	ASN	-	expression tag	UNP Q6UN15-4
F	129	ALA	-	expression tag	UNP Q6UN15-4
H	127	SER	-	expression tag	UNP Q6UN15-4
H	128	ASN	-	expression tag	UNP Q6UN15-4
H	129	ALA	-	expression tag	UNP Q6UN15-4
I	127	SER	-	expression tag	UNP Q6UN15-4
I	128	ASN	-	expression tag	UNP Q6UN15-4
I	129	ALA	-	expression tag	UNP Q6UN15-4
K	127	SER	-	expression tag	UNP Q6UN15-4
K	128	ASN	-	expression tag	UNP Q6UN15-4
K	129	ALA	-	expression tag	UNP Q6UN15-4
L	127	SER	-	expression tag	UNP Q6UN15-4
L	128	ASN	-	expression tag	UNP Q6UN15-4
L	129	ALA	-	expression tag	UNP Q6UN15-4

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	J	2	Total Zn 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	4	Total O 4 4	0	0
4	C	13	Total O 13 13	0	0
4	D	6	Total O 6 6	0	0
4	E	7	Total O 7 7	0	0
4	F	8	Total O 8 8	0	0
4	G	9	Total O 9 9	0	0
4	H	4	Total O 4 4	0	0
4	I	9	Total O 9 9	0	0
4	J	10	Total O 10 10	0	0
4	K	9	Total O 9 9	0	0
4	L	13	Total O 13 13	0	0

3 Residue-property plots (i)

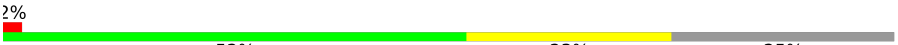
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

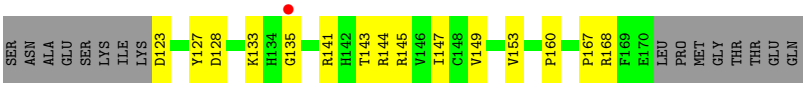
• Molecule 1: Cleavage and polyadenylation specificity factor subunit 4

Chain A:

• Molecule 1: Cleavage and polyadenylation specificity factor subunit 4

Chain D:



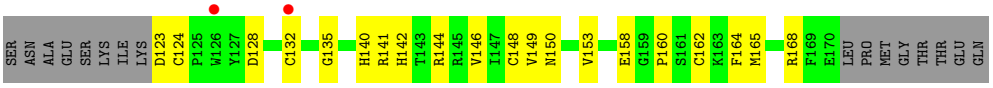


• Molecule 1: Cleavage and polyadenylation specificity factor subunit 4

Chain G:

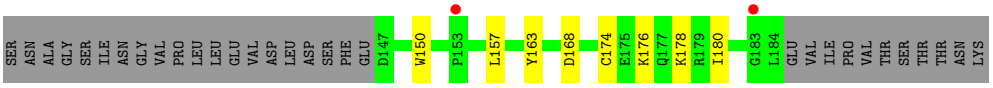
• Molecule 1: Cleavage and polyadenylation specificity factor subunit 4

Chain J:



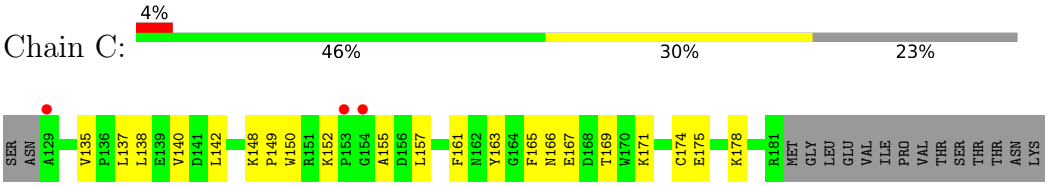
• Molecule 2: Isoform 4 of Pre-mRNA 3'-end-processing factor FIP1

Chain B:



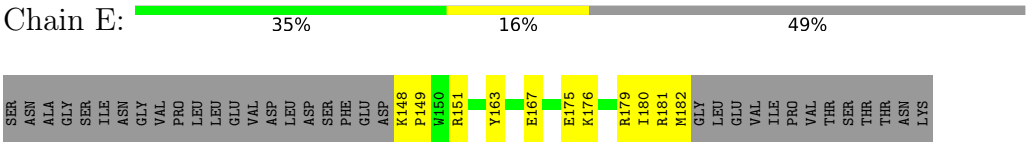
• Molecule 2: Isoform 4 of Pre-mRNA 3'-end-processing factor FIP1

Chain C:



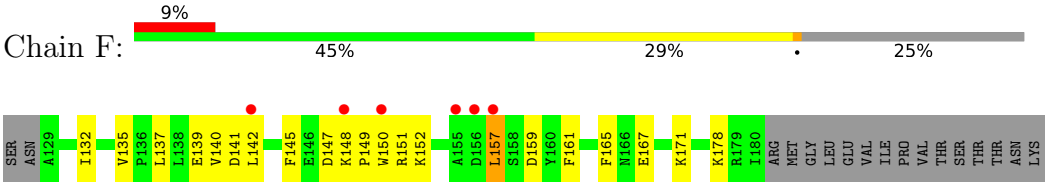
• Molecule 2: Isoform 4 of Pre-mRNA 3'-end-processing factor FIP1

Chain E:



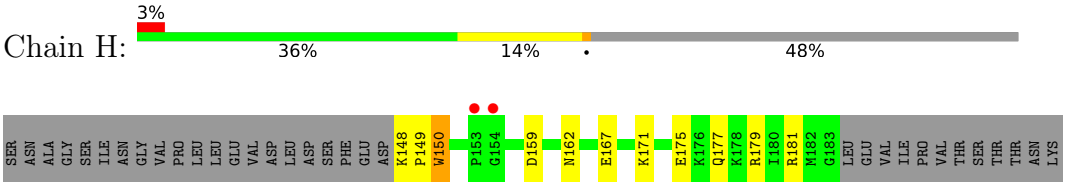
• Molecule 2: Isoform 4 of Pre-mRNA 3'-end-processing factor FIP1

Chain F:



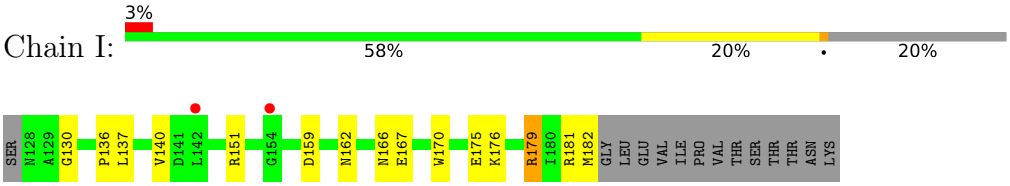
• Molecule 2: Isoform 4 of Pre-mRNA 3'-end-processing factor FIP1

Chain H:



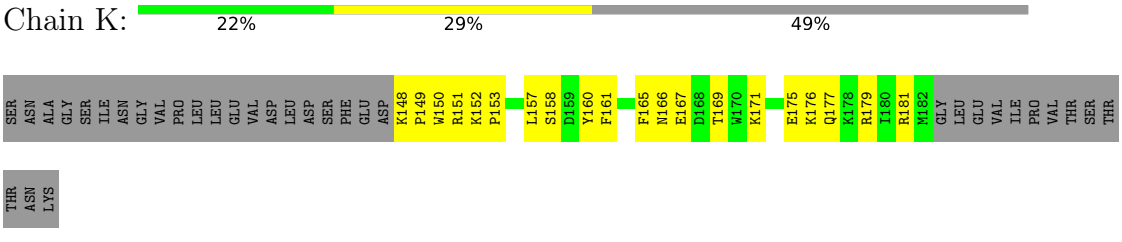
• Molecule 2: Isoform 4 of Pre-mRNA 3'-end-processing factor FIP1

Chain I:



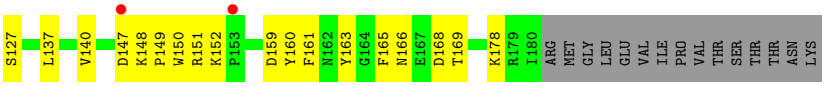
• Molecule 2: Isoform 4 of Pre-mRNA 3'-end-processing factor FIP1

Chain K:



• Molecule 2: Isoform 4 of Pre-mRNA 3'-end-processing factor FIP1

Chain L:


S127
L137
V140
D147
K148
P149
W150
R151
K152
P153
D159
Y160
F161
N162
Y163
G164
F165
N166
E167
D168
T169
K178
R179
I180
ARG
MET
GLY
LEU
GLU
VAL
ILE
PRO
VAL
THR
SER
THR
THR
ASN
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.13Å 115.12Å 66.44Å 90.00° 116.78° 90.00°	Depositor
Resolution (Å)	48.65 – 2.20 48.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.5 (48.65-2.20) 91.7 (48.65-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.247 , 0.264 0.245 , 0.261	Depositor DCC
R_{free} test set	1885 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9075	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1863e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.35	0/426	0.67	0/573
1	D	0.34	0/417	0.64	0/562
1	G	0.36	0/425	0.63	0/572
1	J	0.36	0/417	0.65	0/562
2	B	0.73	2/336 (0.6%)	0.70	0/450
2	C	0.38	0/449	0.63	0/606
2	E	0.39	0/316	0.61	0/423
2	F	0.42	0/438	0.62	0/592
2	H	0.40	0/320	0.64	0/428
2	I	0.40	0/465	0.62	1/627 (0.2%)
2	K	0.35	0/316	0.61	0/423
2	L	0.40	0/452	0.57	0/611
All	All	0.41	2/4777 (0.0%)	0.63	1/6429 (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	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	168	ASP	CB-CG	-9.95	1.30	1.51
2	B	168	ASP	CA-CB	-5.01	1.43	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	179	ARG	CD-NE-CZ	-5.22	116.30	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	168	ARG	Sidechain

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	410	386	386	7	0
1	D	401	373	373	12	0
1	G	409	391	391	11	0
1	J	401	373	373	16	0
2	B	326	308	308	6	0
2	C	437	410	410	18	0
2	E	306	290	290	10	0
2	F	426	397	397	20	0
2	H	310	293	293	11	0
2	I	453	425	425	14	0
2	K	306	290	290	23	0
2	L	440	408	408	16	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
3	G	2	0	0	0	0
3	J	2	0	0	0	0
4	A	6	0	0	0	0
4	B	4	0	0	0	0
4	C	13	0	0	0	0
4	D	6	0	0	0	0
4	E	7	0	0	0	0
4	F	8	0	0	0	0
4	G	9	0	0	0	0
4	H	4	0	0	0	0
4	I	9	0	0	0	0
4	J	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	9	0	0	0	0
4	L	13	0	0	0	0
All	All	4731	4344	4344	143	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 16.

All (143) 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)
2:F:151:ARG:NH2	2:F:167:GLU:OE2	2.05	0.89
1:J:168:ARG:NH2	2:L:159:ASP:OD1	2.07	0.86
2:I:176:LYS:HD2	2:I:179:ARG:NH2	1.96	0.80
2:H:148:LYS:HB3	2:H:149:PRO:CD	2.13	0.78
2:F:141:ASP:HA	2:F:171:LYS:HE2	1.64	0.78
1:A:160:PRO:HB2	1:G:160:PRO:HB3	1.69	0.74
2:E:176:LYS:HE2	2:E:180:ILE:HD11	1.72	0.71
1:D:149:VAL:O	1:D:153:VAL:HG23	1.91	0.71
2:K:148:LYS:CB	2:K:149:PRO:HD3	2.20	0.71
2:L:166:ASN:OD1	2:L:168:ASP:N	2.26	0.69
2:C:152:LYS:HB2	2:C:155:ALA:HB2	1.75	0.68
2:B:150:TRP:HB2	2:B:157:LEU:HD23	1.76	0.67
1:D:145:ARG:HH12	2:L:152:LYS:HE3	1.59	0.66
1:J:148:CYS:HB2	1:J:164:PHE:HB2	1.78	0.66
2:K:148:LYS:HB2	2:K:149:PRO:HD3	1.76	0.66
2:E:148:LYS:HB3	2:E:149:PRO:CD	2.26	0.65
2:H:148:LYS:HB3	2:H:149:PRO:HD2	1.77	0.65
1:D:168:ARG:NH2	2:F:159:ASP:OD1	2.29	0.64
1:G:149:VAL:O	1:G:153:VAL:HG23	1.98	0.64
2:I:166:ASN:OD1	2:I:167:GLU:N	2.31	0.64
2:E:175:GLU:OE2	2:E:179:ARG:NH2	2.31	0.64
2:F:142:LEU:HD13	2:F:171:LYS:HE3	1.79	0.63
2:K:165:PHE:HD1	2:K:169:THR:HG23	1.62	0.63
1:D:128:ASP:O	2:E:163:TYR:OH	2.15	0.62
2:H:177:GLN:OE1	2:H:181:ARG:NH1	2.31	0.62
1:J:124:CYS:HB2	1:J:140:HIS:HB2	1.80	0.62
2:K:176:LYS:HA	2:K:179:ARG:HG3	1.81	0.62
1:G:123:ASP:HA	1:G:141:ARG:HG2	1.80	0.61
2:K:166:ASN:OD1	2:K:169:THR:HG22	2.01	0.60
1:G:153:VAL:HG21	2:I:130:GLY:N	2.16	0.60
1:G:166:HIS:ND1	2:I:159:ASP:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:161:PHE:HB3	2:C:165:PHE:HB2	1.84	0.59
2:I:176:LYS:HD2	2:I:179:ARG:HH21	1.68	0.58
1:J:165:MET:HE3	1:J:165:MET:HA	1.85	0.58
2:E:148:LYS:HB3	2:E:149:PRO:HD2	1.86	0.57
1:D:123:ASP:HA	1:D:141:ARG:HB2	1.86	0.57
2:L:166:ASN:ND2	2:L:169:THR:HG23	2.19	0.57
1:G:148:CYS:HB2	1:G:164:PHE:HB2	1.87	0.57
2:K:148:LYS:CB	2:K:149:PRO:CD	2.83	0.56
2:B:176:LYS:HD3	2:C:163:TYR:OH	2.05	0.56
2:K:157:LEU:HD21	2:K:166:ASN:HA	1.86	0.56
2:F:137:LEU:O	2:F:140:VAL:HG22	2.06	0.56
2:F:142:LEU:HD23	2:F:150:TRP:CE2	2.39	0.56
2:F:139:GLU:HA	2:F:178:LYS:HE2	1.88	0.55
2:C:166:ASN:H	2:C:169:THR:HB	1.71	0.55
2:F:148:LYS:HE2	2:F:151:ARG:NH2	2.21	0.55
2:K:166:ASN:H	2:K:169:THR:CG2	2.20	0.55
2:K:166:ASN:H	2:K:169:THR:HG22	1.72	0.55
1:J:132:CYS:HB3	1:J:142:HIS:CE1	2.42	0.54
1:D:123:ASP:OD2	1:D:143:THR:OG1	2.16	0.54
1:J:123:ASP:HB3	1:J:141:ARG:H	1.72	0.54
2:C:137:LEU:O	2:C:140:VAL:HG22	2.07	0.54
1:G:123:ASP:OD1	1:G:141:ARG:NE	2.40	0.54
2:L:148:LYS:HE2	2:L:151:ARG:CZ	2.38	0.53
1:G:153:VAL:HG21	2:I:130:GLY:H	1.73	0.53
2:F:142:LEU:H	2:F:171:LYS:CE	2.22	0.53
2:C:148:LYS:N	2:C:149:PRO:HD3	2.23	0.52
2:H:167:GLU:HG2	2:H:171:LYS:HZ3	1.74	0.52
2:F:132:ILE:O	2:F:135:VAL:HG22	2.09	0.52
2:K:177:GLN:O	2:K:181:ARG:HG3	2.09	0.52
2:H:175:GLU:O	2:H:179:ARG:HG3	2.10	0.52
1:J:144:ARG:HD3	2:K:158:SER:HB2	1.91	0.52
2:C:149:PRO:HD2	2:C:150:TRP:CZ3	2.46	0.51
1:A:165:MET:HA	1:A:165:MET:HE2	1.93	0.51
1:D:160:PRO:CB	1:J:160:PRO:HB2	2.40	0.51
2:L:147:ASP:OD1	2:L:148:LYS:N	2.40	0.51
2:L:137:LEU:O	2:L:140:VAL:HG22	2.11	0.51
2:E:175:GLU:O	2:E:179:ARG:HG3	2.12	0.50
2:H:167:GLU:O	2:H:171:LYS:HG3	2.11	0.50
2:H:148:LYS:HB3	2:H:149:PRO:HD3	1.93	0.50
2:I:137:LEU:O	2:I:140:VAL:HG22	2.12	0.50
2:I:166:ASN:O	2:I:170:TRP:N	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:148:LYS:HB2	2:K:149:PRO:CD	2.40	0.49
2:L:166:ASN:HD21	2:L:169:THR:HG23	1.76	0.49
2:F:142:LEU:HD23	2:F:150:TRP:CZ2	2.48	0.49
2:C:171:LYS:O	2:C:175:GLU:HG3	2.13	0.49
2:F:147:ASP:HB2	2:F:149:PRO:HD3	1.95	0.49
1:A:143:THR:HG21	1:A:145:ARG:NH1	2.28	0.48
2:F:161:PHE:HB3	2:F:165:PHE:HB2	1.95	0.48
2:K:148:LYS:HB3	2:K:149:PRO:HD3	1.93	0.48
2:F:152:LYS:HB3	2:F:152:LYS:HZ3	1.79	0.48
2:L:161:PHE:HB3	2:L:165:PHE:HB2	1.97	0.47
2:E:181:ARG:O	2:E:182:MET:HB2	2.15	0.47
1:D:133:LYS:N	1:D:133:LYS:HD3	2.30	0.47
1:J:146:VAL:O	1:J:165:MET:HG2	2.15	0.47
2:K:167:GLU:OE2	2:K:171:LYS:NZ	2.47	0.47
2:K:161:PHE:HB3	2:K:165:PHE:HB2	1.97	0.47
2:E:181:ARG:O	2:E:182:MET:CB	2.63	0.46
2:F:142:LEU:CD1	2:F:171:LYS:HE3	2.43	0.46
2:F:152:LYS:HE3	1:J:165:MET:HE1	1.97	0.45
1:J:158:GLU:HB2	1:J:162:CYS:HB2	1.99	0.45
1:D:167:PRO:HG3	2:E:163:TYR:CZ	2.52	0.45
1:A:155:PHE:O	2:C:137:LEU:HD21	2.17	0.45
1:D:147:ILE:HG13	1:D:167:PRO:CD	2.47	0.45
2:L:149:PRO:HB2	2:L:160:TYR:OH	2.16	0.45
1:J:135:GLY:HA2	1:J:142:HIS:CE1	2.51	0.45
2:K:152:LYS:HG3	2:K:153:PRO:HD2	1.99	0.44
2:I:136:PRO:O	2:I:140:VAL:HG13	2.18	0.44
2:H:148:LYS:CB	2:H:149:PRO:CD	2.85	0.44
2:I:151:ARG:NH2	2:I:167:GLU:OE2	2.51	0.44
2:L:178:LYS:C	2:L:178:LYS:HD3	2.37	0.44
2:C:135:VAL:HG12	2:C:140:VAL:HG12	1.99	0.44
2:H:148:LYS:HB2	2:H:150:TRP:CZ2	2.53	0.43
1:J:149:VAL:HG22	2:L:127:SER:OG	2.18	0.43
2:H:148:LYS:HD3	2:H:150:TRP:CH2	2.54	0.43
2:K:149:PRO:HD2	2:K:150:TRP:CZ3	2.53	0.43
1:J:135:GLY:HA2	1:J:142:HIS:HE1	1.84	0.42
2:K:149:PRO:HD2	2:K:150:TRP:CE3	2.53	0.42
2:C:174:CYS:O	2:C:178:LYS:HG3	2.18	0.42
1:G:151:TYR:O	2:I:162:ASN:HB2	2.19	0.42
2:C:138:LEU:O	2:C:178:LYS:HE2	2.20	0.42
2:I:175:GLU:O	2:I:179:ARG:HG3	2.20	0.42
2:L:148:LYS:N	2:L:149:PRO:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:MET:HG3	2:B:163:TYR:HE1	1.85	0.42
1:G:127:TYR:O	2:H:162:ASN:HB2	2.20	0.42
2:C:149:PRO:HD2	2:C:150:TRP:CE3	2.54	0.42
2:K:167:GLU:HG2	2:K:171:LYS:HZ3	1.85	0.42
2:K:151:ARG:O	2:K:151:ARG:HG2	2.20	0.42
1:J:150:ASN:HA	1:J:153:VAL:HG12	2.02	0.42
1:D:127:TYR:OH	1:D:144:ARG:HG2	2.19	0.42
2:I:181:ARG:O	2:I:182:MET:HG2	2.20	0.42
2:L:149:PRO:HD2	2:L:150:TRP:CE3	2.55	0.41
2:F:157:LEU:HD23	2:F:161:PHE:HD2	1.85	0.41
2:B:174:CYS:O	2:B:178:LYS:HG3	2.20	0.41
2:F:149:PRO:HD2	2:F:150:TRP:CE3	2.55	0.41
2:K:149:PRO:HG2	2:K:160:TYR:CE2	2.55	0.41
2:B:176:LYS:HG2	2:B:180:ILE:HD12	2.02	0.41
2:F:152:LYS:HB3	2:F:152:LYS:NZ	2.35	0.41
2:L:166:ASN:H	2:L:169:THR:HG1	1.64	0.41
2:C:150:TRP:HB2	2:C:157:LEU:CD2	2.50	0.41
2:K:176:LYS:HD3	2:L:163:TYR:OH	2.21	0.41
1:A:122:LYS:O	1:A:141:ARG:HD2	2.21	0.41
2:C:142:LEU:H	2:C:142:LEU:HD12	1.86	0.41
2:E:151:ARG:NH2	2:E:167:GLU:OE1	2.54	0.41
2:K:175:GLU:O	2:K:179:ARG:CG	2.69	0.41
2:B:180:ILE:HG22	2:C:163:TYR:HB3	2.02	0.40
2:C:142:LEU:HD13	2:C:171:LYS:HG2	2.03	0.40
2:F:142:LEU:HA	2:F:145:PHE:HD2	1.86	0.40
2:C:150:TRP:CD1	2:C:167:GLU:OE2	2.75	0.40
1:A:148:CYS:HB2	1:A:164:PHE:HB2	2.03	0.40
1:G:146:VAL:CG2	1:G:164:PHE:HD1	2.35	0.40
2:I:179:ARG:HH11	2:I:179:ARG:HD2	1.55	0.40
1:D:160:PRO:HB2	1:J:160:PRO:HB2	2.03	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	47/64 (73%)	45 (96%)	2 (4%)	0	100	100
1	D	46/64 (72%)	42 (91%)	3 (6%)	1 (2%)	6	4
1	G	47/64 (73%)	43 (92%)	4 (8%)	0	100	100
1	J	46/64 (72%)	44 (96%)	2 (4%)	0	100	100
2	B	36/69 (52%)	36 (100%)	0	0	100	100
2	C	51/69 (74%)	48 (94%)	3 (6%)	0	100	100
2	E	33/69 (48%)	33 (100%)	0	0	100	100
2	F	50/69 (72%)	49 (98%)	1 (2%)	0	100	100
2	H	34/69 (49%)	34 (100%)	0	0	100	100
2	I	53/69 (77%)	51 (96%)	2 (4%)	0	100	100
2	K	33/69 (48%)	32 (97%)	1 (3%)	0	100	100
2	L	52/69 (75%)	51 (98%)	1 (2%)	0	100	100
All	All	528/808 (65%)	508 (96%)	19 (4%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	135	GLY

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	45/58 (78%)	45 (100%)	0	100	100
1	D	44/58 (76%)	44 (100%)	0	100	100
1	G	45/58 (78%)	45 (100%)	0	100	100
1	J	44/58 (76%)	43 (98%)	1 (2%)	50	63
2	B	33/61 (54%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	46/61 (75%)	46 (100%)	0	100 100
2	E	31/61 (51%)	31 (100%)	0	100 100
2	F	45/61 (74%)	44 (98%)	1 (2%)	52 65
2	H	31/61 (51%)	29 (94%)	2 (6%)	17 19
2	I	48/61 (79%)	48 (100%)	0	100 100
2	K	31/61 (51%)	31 (100%)	0	100 100
2	L	47/61 (77%)	47 (100%)	0	100 100
All	All	490/720 (68%)	486 (99%)	4 (1%)	81 90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	157	LEU
2	H	150	TRP
2	H	159	ASP
1	J	128	ASP

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

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	49/64 (76%)	0.26	0 100 100	36, 47, 61, 69	0
1	D	48/64 (75%)	0.44	1 (2%) 63 61	38, 53, 73, 76	0
1	G	49/64 (76%)	0.52	1 (2%) 65 63	41, 55, 71, 84	0
1	J	48/64 (75%)	0.41	2 (4%) 36 34	43, 52, 65, 83	0
2	B	38/69 (55%)	0.33	2 (5%) 26 25	37, 54, 80, 100	0
2	C	53/69 (76%)	0.57	3 (5%) 23 22	41, 54, 84, 115	0
2	E	35/69 (50%)	0.28	0 100 100	43, 55, 78, 91	0
2	F	52/69 (75%)	0.81	6 (11%) 4 4	37, 57, 88, 106	0
2	H	36/69 (52%)	0.50	2 (5%) 24 23	45, 62, 86, 95	0
2	I	55/69 (79%)	0.40	2 (3%) 42 41	43, 54, 86, 97	0
2	K	35/69 (50%)	0.12	0 100 100	39, 47, 64, 68	0
2	L	54/69 (78%)	0.39	2 (3%) 41 39	42, 52, 96, 121	0
All	All	552/808 (68%)	0.43	21 (3%) 40 38	36, 53, 83, 121	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	154	GLY	7.2
2	F	155	ALA	5.6
2	H	153	PRO	5.0
2	I	154	GLY	4.3
1	J	126	TRP	3.8
2	L	147	ASP	3.7
2	L	153	PRO	3.4
2	F	142	LEU	2.8
2	B	153	PRO	2.7
2	C	153	PRO	2.7
2	F	157	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	156	ASP	2.6
2	F	148	LYS	2.6
2	F	150	TRP	2.4
2	C	129	ALA	2.3
2	B	183	GLY	2.3
2	I	142	LEU	2.2
1	D	135	GLY	2.1
2	H	154	GLY	2.1
1	G	139	ARG	2.0
1	J	132	CYS	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	1001	1/1	0.95	0.10	69,69,69,69	0
3	ZN	G	1001	1/1	0.97	0.12	60,60,60,60	0
3	ZN	J	1002	1/1	0.97	0.13	60,60,60,60	0
3	ZN	G	1002	1/1	0.98	0.15	54,54,54,54	0
3	ZN	J	1001	1/1	0.98	0.12	56,56,56,56	0
3	ZN	A	1001	1/1	0.98	0.14	54,54,54,54	0
3	ZN	D	1002	1/1	0.99	0.16	54,54,54,54	0
3	ZN	A	1002	1/1	1.00	0.16	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.