



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:10 pm BST

PDB ID : 6JMT  
Title : Crystal structure of GIT/PIX complex  
Authors : Zhu, J.; Lin, L.; Xia, Y.; Zhang, R.; Zhang, M.  
Deposited on : 2019-03-13  
Resolution : 2.80 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](mailto: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.

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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	:	2.11
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)	:	2.11

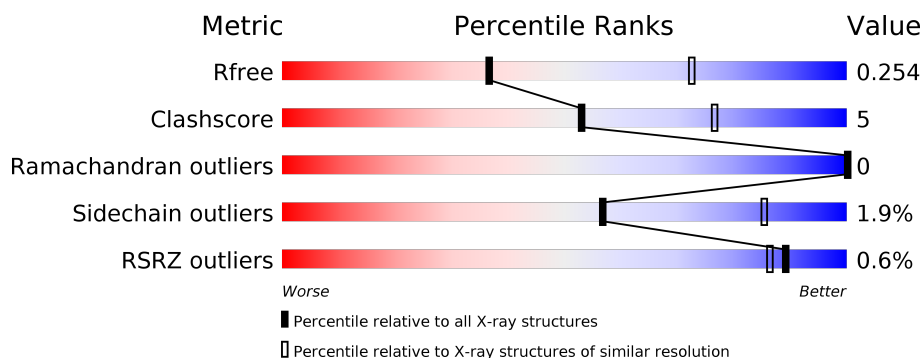
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	364	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	B	364	<div> <div></div> <div>80%</div> <div>15%</div> <div>•</div> </div>
1	C	364	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 7%</div> </div> </div>
1	D	364	<div> <div></div> <div>83%</div> <div>13%</div> <div>•</div> </div>
1	E	364	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
1	F	364	<div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	21	 <div>67%10%24%</div>
2	J	21	 <div>62%14%24%</div>
2	K	21	 <div>67%10%24%</div>
2	L	21	 <div>71%5%24%</div>
2	M	21	 <div>76%0%24%</div>
2	N	21	 <div>62%14%24%</div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16305 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 ARF GTPase-activating protein GIT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2619	1640	479	489	11			
1	D	350	Total	C	N	O	S	0	0	0
			2634	1645	486	491	12			
1	B	349	Total	C	N	O	S	0	0	0
			2650	1655	487	496	12			
1	C	339	Total	C	N	O	S	0	0	0
			2485	1558	460	458	9			
1	E	343	Total	C	N	O	S	0	0	0
			2544	1596	465	472	11			
1	F	346	Total	C	N	O	S	0	0	0
			2625	1639	482	492	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q80XR8
A	-2	PRO	-	expression tag	UNP Q80XR8
A	-1	GLY	-	expression tag	UNP Q80XR8
A	0	SER	-	expression tag	UNP Q80XR8
A	255	ALA	SER	engineered mutation	UNP Q80XR8
A	256	ALA	SER	engineered mutation	UNP Q80XR8
D	-3	GLY	-	expression tag	UNP Q80XR8
D	-2	PRO	-	expression tag	UNP Q80XR8
D	-1	GLY	-	expression tag	UNP Q80XR8
D	0	SER	-	expression tag	UNP Q80XR8
D	255	ALA	SER	engineered mutation	UNP Q80XR8
D	256	ALA	SER	engineered mutation	UNP Q80XR8
B	-3	GLY	-	expression tag	UNP Q80XR8
B	-2	PRO	-	expression tag	UNP Q80XR8
B	-1	GLY	-	expression tag	UNP Q80XR8
B	0	SER	-	expression tag	UNP Q80XR8
B	255	ALA	SER	engineered mutation	UNP Q80XR8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	256	ALA	SER	engineered mutation	UNP Q80XR8
C	-3	GLY	-	expression tag	UNP Q80XR8
C	-2	PRO	-	expression tag	UNP Q80XR8
C	-1	GLY	-	expression tag	UNP Q80XR8
C	0	SER	-	expression tag	UNP Q80XR8
C	255	ALA	SER	engineered mutation	UNP Q80XR8
C	256	ALA	SER	engineered mutation	UNP Q80XR8
E	-3	GLY	-	expression tag	UNP Q80XR8
E	-2	PRO	-	expression tag	UNP Q80XR8
E	-1	GLY	-	expression tag	UNP Q80XR8
E	0	SER	-	expression tag	UNP Q80XR8
E	255	ALA	SER	engineered mutation	UNP Q80XR8
E	256	ALA	SER	engineered mutation	UNP Q80XR8
F	-3	GLY	-	expression tag	UNP Q80XR8
F	-2	PRO	-	expression tag	UNP Q80XR8
F	-1	GLY	-	expression tag	UNP Q80XR8
F	0	SER	-	expression tag	UNP Q80XR8
F	255	ALA	SER	engineered mutation	UNP Q80XR8
F	256	ALA	SER	engineered mutation	UNP Q80XR8

- Molecule 2 is a protein called beta PIX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	16	Total	C	N	O	S	0	0	0
			121	77	17	26	1			
2	J	16	Total	C	N	O	S	0	0	0
			121	77	17	26	1			
2	K	16	Total	C	N	O	S	0	0	0
			125	80	18	26	1			
2	L	16	Total	C	N	O	S	0	0	0
			125	80	18	26	1			
2	M	16	Total	C	N	O	S	0	0	0
			125	80	18	26	1			
2	N	16	Total	C	N	O	S	0	0	0
			125	80	18	26	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		

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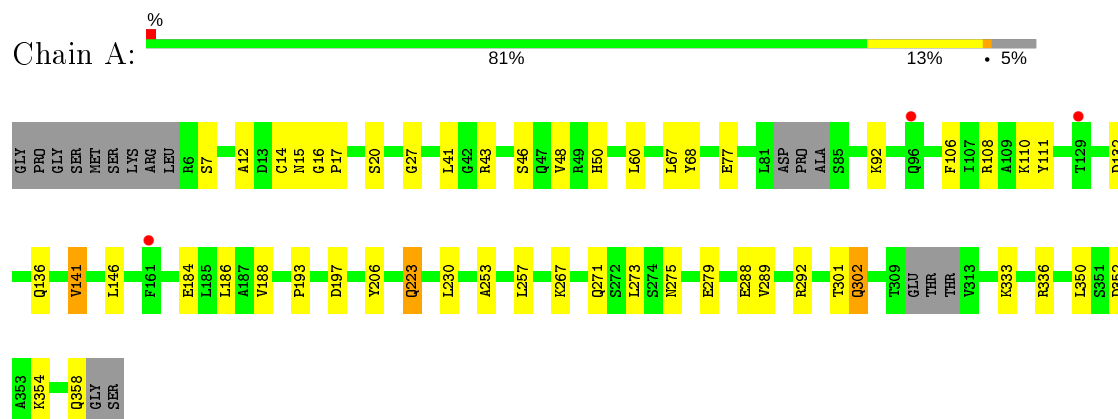
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

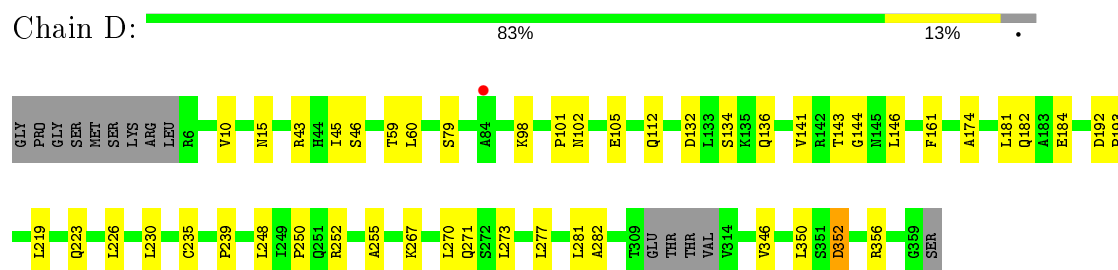
### 3 Residue-property plots [i](#)

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

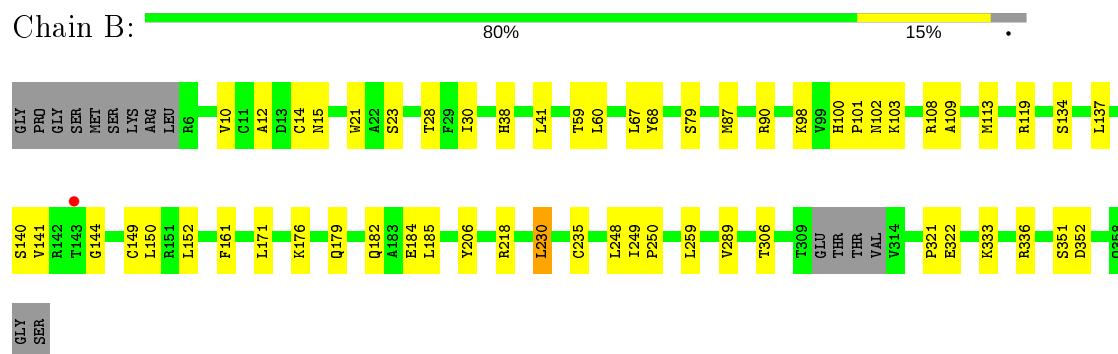
- Molecule 1: ARF GTPase-activating protein GIT2



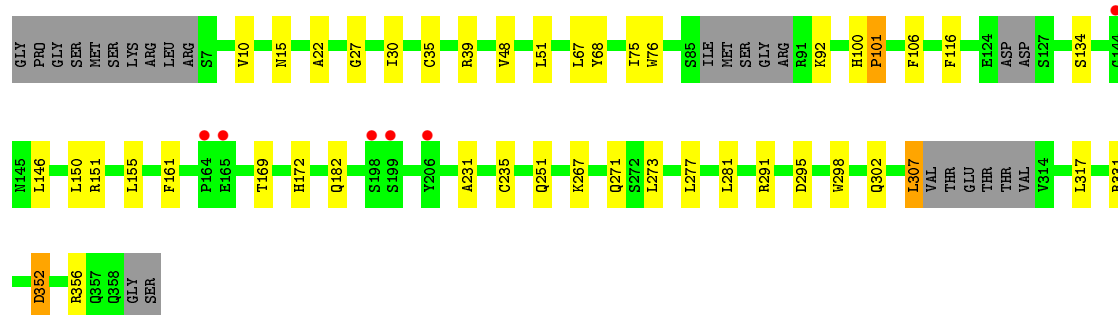
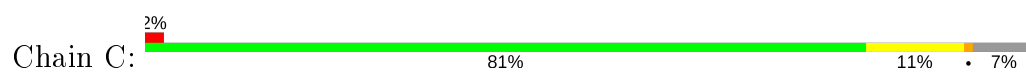
- Molecule 1: ARF GTPase-activating protein GIT2



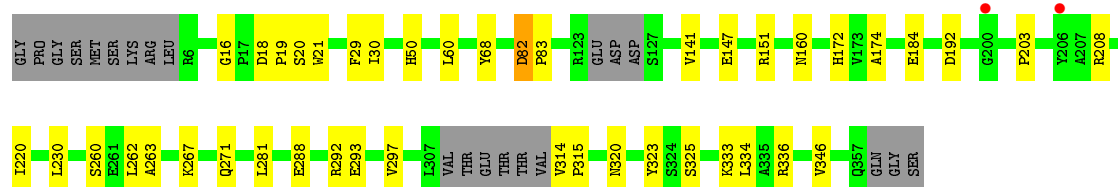
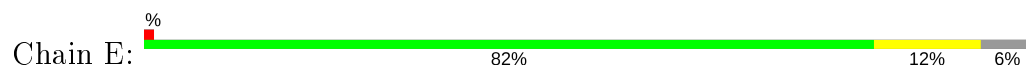
- Molecule 1: ARF GTPase-activating protein GIT2



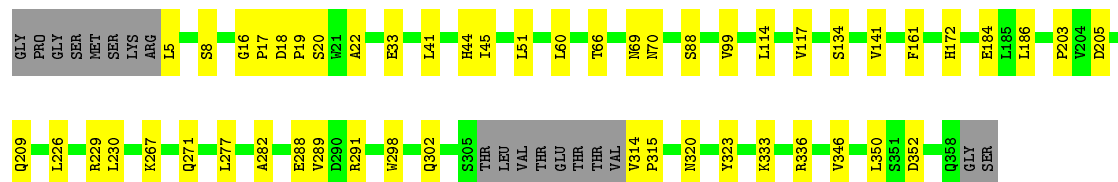
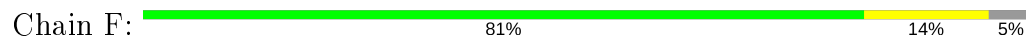
- Molecule 1: ARF GTPase-activating protein GIT2



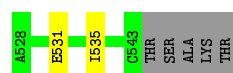
- Molecule 1: ARF GTPase-activating protein GIT2



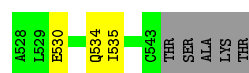
- Molecule 1: ARF GTPase-activating protein GIT2



- Molecule 2: beta PIX



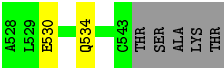
- Molecule 2: beta PIX



- Molecule 2: beta PIX







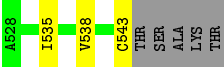
- Molecule 2: beta PIX



- Molecule 2: beta PIX



- Molecule 2: beta PIX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.96 Å   322.68 Å   44.47 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	44.05 – 2.80 44.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (44.05-2.80) 94.8 (44.05-2.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.07 (at 2.81 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.194   ,   0.254 0.196   ,   0.254	Depositor DCC
$R_{free}$ test set	2987 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.49	1/2676 (0.0%)	0.58	1/3642 (0.0%)
1	B	0.51	0/2709	0.59	0/3685
1	C	0.46	1/2539 (0.0%)	0.57	0/3466
1	D	0.48	0/2693	0.58	0/3666
1	E	0.46	0/2601	0.58	2/3548 (0.1%)
1	F	0.50	2/2684 (0.1%)	0.62	2/3652 (0.1%)
2	I	0.44	0/121	0.46	0/164
2	J	0.44	0/121	0.49	0/164
2	K	0.46	0/125	0.54	0/168
2	L	0.46	0/125	0.49	0/168
2	M	0.54	0/125	0.59	0/168
2	N	0.50	0/125	0.54	0/168
All	All	0.48	4/16644 (0.0%)	0.58	5/22659 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	PRO	N-CD	5.43	1.55	1.47
1	F	17	PRO	N-CD	5.17	1.55	1.47
1	A	17	PRO	N-CD	5.17	1.55	1.47
1	F	19	PRO	N-CD	5.03	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	ASP	C-N-CD	5.79	140.57	128.40
1	A	16	GLY	C-N-CD	5.74	140.46	128.40
1	E	16	GLY	C-N-CD	5.63	140.23	128.40
1	F	18	ASP	C-N-CD	5.51	139.97	128.40
1	F	16	GLY	C-N-CD	5.45	139.85	128.40

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	2619	0	2447	30	0
1	B	2650	0	2501	34	0
1	C	2485	0	2271	28	0
1	D	2634	0	2460	30	0
1	E	2544	0	2342	23	0
1	F	2625	0	2468	26	0
2	I	121	0	113	2	0
2	J	121	0	113	2	0
2	K	125	0	124	1	0
2	L	125	0	124	1	0
2	M	125	0	124	0	0
2	N	125	0	124	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	16305	0	15211	170	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 5.

All (170) 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:E:147:GLU:OE2	1:E:151:ARG:NH1	2.15	0.80
1:A:275:ASN:O	1:A:279:GLU:HG3	1.82	0.79
1:A:197:ASP:OD2	1:A:206:TYR:OH	2.01	0.78
1:F:60:LEU:HA	1:F:184:GLU:HG2	1.71	0.71
1:E:333:LYS:HA	1:E:336:ARG:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LEU:HD12	1:C:331:ARG:HB3	1.73	0.69
1:D:60:LEU:HA	1:D:184:GLU:HG2	1.75	0.69
1:E:60:LEU:HA	1:E:184:GLU:HG2	1.73	0.69
1:A:60:LEU:HA	1:A:184:GLU:HG2	1.76	0.66
1:C:277:LEU:HD21	2:I:531:GLU:HB3	1.78	0.65
1:C:231:ALA:O	1:C:235:CYS:HB2	1.96	0.64
1:A:14:CYS:O	1:A:15:ASN:HB2	1.96	0.64
2:K:530:GLU:OE2	2:K:534:GLN:NE2	2.30	0.64
1:A:67:LEU:HD13	1:A:146:LEU:HB3	1.80	0.64
1:D:352:ASP:OD2	1:D:356:ARG:NH1	2.30	0.64
1:D:10:VAL:HG13	1:D:15:ASN:HA	1.80	0.63
1:D:101:PRO:O	1:D:105:GLU:HG3	1.99	0.63
1:A:267:LYS:O	1:A:271:GLN:HG3	1.99	0.63
1:F:66:THR:O	1:F:70:ASN:ND2	2.33	0.61
1:D:45:ILE:HD13	1:D:112:GLN:HG3	1.83	0.60
1:B:59:THR:HG23	1:B:184:GLU:OE2	2.02	0.60
1:C:39:ARG:NH2	1:C:295:ASP:OD1	2.32	0.60
1:C:10:VAL:HG13	1:C:15:ASN:HA	1.84	0.59
1:D:273:LEU:HD11	2:N:538:VAL:HG21	1.85	0.59
1:A:302:GLN:HE21	1:A:302:GLN:N	2.01	0.58
1:C:281:LEU:HD13	2:I:535:ILE:HG23	1.85	0.58
1:B:10:VAL:HG13	1:B:15:ASN:HA	1.86	0.57
1:D:239:PRO:HG3	1:D:248:LEU:HB2	1.85	0.57
1:A:273:LEU:HD11	2:L:538:VAL:HG21	1.87	0.56
1:F:134:SER:HB3	1:F:161:PHE:CD2	2.39	0.56
1:C:267:LYS:O	1:C:271:GLN:HG3	2.06	0.56
1:F:5:LEU:HA	1:F:69:ASN:ND2	2.20	0.56
1:A:193:PRO:HB2	1:A:223:GLN:HG3	1.88	0.55
1:B:23:SER:HB3	1:B:28:THR:HG22	1.89	0.55
1:B:60:LEU:HA	1:B:184:GLU:HG2	1.89	0.55
1:A:50:HIS:CD2	1:A:301:THR:HG21	2.43	0.54
1:B:109:ALA:HA	1:B:113:MET:HB2	1.89	0.54
1:B:179:GLN:HB3	1:B:182:GLN:HG3	1.89	0.54
1:F:267:LYS:O	1:F:271:GLN:HG3	2.08	0.54
1:A:77:GLU:HG3	1:A:110:LYS:HE3	1.89	0.54
1:F:141:VAL:HG11	1:F:186:LEU:HD11	1.90	0.53
1:C:92:LYS:HG3	1:C:106:PHE:CE2	2.44	0.53
1:D:267:LYS:O	1:D:271:GLN:HG3	2.09	0.53
1:A:230:LEU:HD22	1:A:289:VAL:HG21	1.90	0.53
1:C:271:GLN:HG2	1:C:352:ASP:OD2	2.09	0.53
1:C:273:LEU:O	1:C:356:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLY:O	1:B:182:GLN:NE2	2.43	0.52
1:D:143:THR:HG22	1:D:144:GLY:N	2.24	0.52
1:A:302:GLN:NE2	1:A:302:GLN:CA	2.73	0.52
1:C:298:TRP:HE1	1:C:307:LEU:HD11	1.75	0.51
1:E:160:ASN:HD21	1:E:192:ASP:HB2	1.74	0.51
1:D:230:LEU:HD13	1:D:346:VAL:HG13	1.92	0.51
1:E:267:LYS:O	1:E:271:GLN:HG3	2.11	0.51
1:B:98:LYS:O	1:B:102:ASN:HB2	2.11	0.51
1:F:333:LYS:O	1:F:336:ARG:HG2	2.10	0.51
1:A:92:LYS:HG3	1:A:106:PHE:CZ	2.46	0.50
1:E:260:SER:HB2	1:E:263:ALA:H	1.77	0.49
1:D:45:ILE:CD1	1:D:112:GLN:HG3	2.41	0.49
1:B:59:THR:HG21	1:B:218:ARG:HG2	1.94	0.49
1:D:235:CYS:SG	1:D:250:PRO:HB3	2.53	0.49
1:D:143:THR:HG22	1:D:144:GLY:H	1.78	0.49
1:D:193:PRO:HB2	1:D:223:GLN:HG3	1.95	0.48
1:A:43:ARG:HA	1:A:46:SER:O	2.14	0.48
1:C:67:LEU:HD13	1:C:146:LEU:HB3	1.96	0.48
1:E:230:LEU:HB3	1:E:346:VAL:HG13	1.94	0.48
1:B:23:SER:HB3	1:B:28:THR:CG2	2.43	0.48
1:D:134:SER:HB3	1:D:161:PHE:CG	2.48	0.47
2:J:530:GLU:O	2:J:534:GLN:HG3	2.14	0.47
1:C:76:TRP:O	1:C:116:PHE:HB2	2.14	0.47
1:B:14:CYS:CB	1:B:103:LYS:HE2	2.45	0.47
1:A:141:VAL:HG21	1:A:186:LEU:HD11	1.96	0.47
1:C:169:THR:O	1:C:172:HIS:HB2	2.15	0.47
1:F:298:TRP:O	1:F:302:GLN:HG2	2.14	0.47
1:F:33:GLU:HB3	1:F:99:VAL:HG22	1.95	0.47
1:B:176:LYS:HE2	1:B:206:TYR:CE1	2.49	0.47
1:B:321:PRO:HB2	1:F:88:SER:HB3	1.97	0.47
1:E:288:GLU:OE1	1:E:292:ARG:NH1	2.47	0.47
1:C:22:ALA:HB2	1:C:51:LEU:HD21	1.96	0.46
1:A:288:GLU:HG3	1:A:292:ARG:HD2	1.98	0.46
1:B:38:HIS:HA	1:B:41:LEU:HD12	1.98	0.46
1:D:146:LEU:HD11	1:D:181:LEU:HB3	1.98	0.46
1:C:291:ARG:HD3	1:C:317:LEU:HD23	1.97	0.46
1:D:98:LYS:O	1:D:102:ASN:HB2	2.16	0.46
1:A:184:GLU:O	1:A:188:VAL:HG23	2.16	0.46
1:A:302:GLN:NE2	1:A:302:GLN:N	2.64	0.45
1:C:317:LEU:HD13	1:C:331:ARG:NH2	2.31	0.45
1:B:248:LEU:O	1:B:250:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:O	1:A:136:GLN:HG3	2.17	0.45
1:F:22:ALA:HB2	1:F:51:LEU:HD21	1.98	0.45
1:A:12:ALA:O	1:A:110:LYS:NZ	2.50	0.45
1:A:41:LEU:HD21	1:A:108:ARG:HG2	1.99	0.45
1:C:67:LEU:HD21	1:C:150:LEU:HD22	1.99	0.45
1:E:208:ARG:HH21	1:E:220:ILE:HD11	1.81	0.45
1:E:60:LEU:HA	1:E:184:GLU:CG	2.46	0.45
1:B:41:LEU:HD21	1:B:108:ARG:HG2	1.99	0.45
1:F:41:LEU:HD13	1:F:45:ILE:HG21	1.98	0.45
1:C:298:TRP:O	1:C:302:GLN:HG2	2.17	0.44
1:C:27:GLY:O	1:C:68:TYR:HB2	2.18	0.44
1:F:277:LEU:HD23	1:F:277:LEU:HA	1.81	0.44
1:E:320:ASN:HB3	1:E:323:TYR:CD2	2.53	0.44
1:B:249:ILE:HD12	1:B:351:SER:HA	1.99	0.44
1:D:141:VAL:HG13	1:D:182:GLN:HB3	1.98	0.44
1:E:29:PHE:HB2	1:E:68:TYR:CE2	2.53	0.44
1:B:100:HIS:HA	1:B:101:PRO:HA	1.82	0.44
1:C:30:ILE:HD12	1:C:35:CYS:HA	2.00	0.44
1:D:141:VAL:CG1	1:D:174:ALA:HB2	2.48	0.44
1:F:172:HIS:NE2	1:F:203:PRO:HD3	2.33	0.44
1:F:205:ASP:O	1:F:209:GLN:HG3	2.18	0.44
1:A:336:ARG:HH11	1:A:336:ARG:HG2	1.81	0.44
1:B:137:LEU:O	1:B:141:VAL:HG13	2.18	0.44
1:C:298:TRP:NE1	1:C:307:LEU:HD11	2.33	0.44
1:A:333:LYS:O	1:A:336:ARG:HG3	2.18	0.43
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.84	0.43
1:A:27:GLY:O	1:A:68:TYR:HB2	2.18	0.43
1:E:281:LEU:HD13	2:J:535:ILE:HG23	2.00	0.43
1:A:354:LYS:O	1:A:358:GLN:HG3	2.17	0.43
1:D:134:SER:HB3	1:D:161:PHE:CD2	2.53	0.43
1:D:43:ARG:HA	1:D:46:SER:O	2.18	0.43
1:A:110:LYS:HD3	1:A:111:TYR:CE2	2.53	0.43
1:B:230:LEU:HD22	1:B:289:VAL:HG21	1.99	0.43
1:F:134:SER:HB3	1:F:161:PHE:CG	2.54	0.43
1:F:288:GLU:OE1	1:F:291:ARG:NH1	2.51	0.43
1:D:281:LEU:HD13	2:N:535:ILE:HG23	2.00	0.43
1:A:253:ALA:HB1	1:B:250:PRO:HB3	2.01	0.43
1:B:134:SER:HB3	1:B:161:PHE:CG	2.54	0.42
1:B:79:SER:OG	1:B:90:ARG:NH1	2.52	0.42
1:D:226:LEU:HD21	1:D:282:ALA:HB1	2.02	0.42
1:D:277:LEU:HD23	1:D:277:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:HIS:NE2	1:E:203:PRO:HD3	2.34	0.42
1:C:134:SER:HB3	1:C:161:PHE:CG	2.54	0.42
1:C:151:ARG:O	1:C:155:LEU:HG	2.20	0.42
1:E:160:ASN:HD21	1:E:192:ASP:CB	2.31	0.42
1:F:230:LEU:HB3	1:F:346:VAL:HG13	2.02	0.42
1:D:252:ARG:NH1	1:D:255:ALA:HA	2.35	0.42
1:B:333:LYS:O	1:B:336:ARG:HG2	2.20	0.42
1:F:320:ASN:HB3	1:F:323:TYR:CD2	2.54	0.42
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.81	0.42
1:A:230:LEU:HB2	1:A:350:LEU:HD21	2.02	0.42
1:F:350:LEU:HA	1:F:350:LEU:HD23	1.83	0.42
1:E:82:ASP:HA	1:E:83:PRO:HD3	1.83	0.42
1:A:12:ALA:HB2	1:A:68:TYR:CE1	2.55	0.41
1:B:12:ALA:HB2	1:B:68:TYR:CE1	2.55	0.41
1:C:134:SER:HB3	1:C:161:PHE:CD2	2.55	0.41
1:D:132:ASP:O	1:D:136:GLN:HG3	2.19	0.41
1:E:293:GLU:O	1:E:297:VAL:HG23	2.20	0.41
1:D:277:LEU:HD22	2:N:535:ILE:HD11	2.03	0.41
1:B:322:GLU:OE1	1:F:88:SER:OG	2.35	0.41
1:F:314:VAL:N	1:F:315:PRO:HD3	2.36	0.41
1:B:21:TRP:HB2	1:B:30:ILE:HG13	2.03	0.41
1:E:21:TRP:CE2	1:E:50:HIS:HD2	2.39	0.41
1:C:100:HIS:HA	1:C:101:PRO:HA	1.66	0.41
1:E:141:VAL:HG13	1:E:174:ALA:HB2	2.03	0.41
1:C:298:TRP:CE2	1:C:302:GLN:HG3	2.56	0.41
1:F:226:LEU:HD21	1:F:282:ALA:HB1	2.02	0.41
1:C:75:ILE:HD11	1:C:151:ARG:HB2	2.02	0.40
1:D:350:LEU:HA	1:D:350:LEU:HD23	1.89	0.40
1:E:262:LEU:HD23	1:E:262:LEU:HA	1.95	0.40
1:E:334:LEU:HA	1:E:334:LEU:HD23	1.97	0.40
1:B:152:LEU:HD23	1:B:152:LEU:HA	1.78	0.40
1:B:14:CYS:O	1:B:15:ASN:HB2	2.22	0.40
1:B:67:LEU:HD21	1:B:150:LEU:HD22	2.03	0.40
1:E:19:PRO:HB2	1:E:30:ILE:O	2.22	0.40
1:E:314:VAL:HA	1:E:315:PRO:HD3	1.83	0.40
1:F:44:HIS:CE1	1:F:320:ASN:HA	2.56	0.40
1:B:149:CYS:SG	1:B:185:LEU:HD23	2.62	0.40
1:B:235:CYS:SG	1:B:250:PRO:HG3	2.62	0.40
1:F:229:ARG:HH21	1:F:289:VAL:HG12	1.85	0.40
1:B:87:MET:HG3	1:B:90:ARG:HG3	2.03	0.40
1:D:192:ASP:HA	1:D:193:PRO:HD3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:LEU:O	1:F:117:VAL:HG22	2.22	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	341/364 (94%)	337 (99%)	4 (1%)	0	100	100
1	B	345/364 (95%)	335 (97%)	10 (3%)	0	100	100
1	C	331/364 (91%)	320 (97%)	11 (3%)	0	100	100
1	D	346/364 (95%)	340 (98%)	6 (2%)	0	100	100
1	E	337/364 (93%)	330 (98%)	7 (2%)	0	100	100
1	F	342/364 (94%)	336 (98%)	6 (2%)	0	100	100
2	I	14/21 (67%)	14 (100%)	0	0	100	100
2	J	14/21 (67%)	14 (100%)	0	0	100	100
2	K	14/21 (67%)	14 (100%)	0	0	100	100
2	L	14/21 (67%)	14 (100%)	0	0	100	100
2	M	14/21 (67%)	14 (100%)	0	0	100	100
2	N	14/21 (67%)	14 (100%)	0	0	100	100
All	All	2126/2310 (92%)	2082 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	262/311 (84%)	254 (97%)	8 (3%)	40	74
1	B	270/311 (87%)	264 (98%)	6 (2%)	52	83
1	C	235/311 (76%)	230 (98%)	5 (2%)	53	84
1	D	263/311 (85%)	259 (98%)	4 (2%)	65	89
1	E	247/311 (79%)	244 (99%)	3 (1%)	71	92
1	F	267/311 (86%)	264 (99%)	3 (1%)	73	92
2	I	12/17 (71%)	12 (100%)	0	100	100
2	J	12/17 (71%)	12 (100%)	0	100	100
2	K	13/17 (76%)	13 (100%)	0	100	100
2	L	13/17 (76%)	13 (100%)	0	100	100
2	M	13/17 (76%)	13 (100%)	0	100	100
2	N	13/17 (76%)	12 (92%)	1 (8%)	13	35
All	All	1620/1968 (82%)	1590 (98%)	30 (2%)	57	85

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	20	SER
1	A	48	VAL
1	A	141	VAL
1	A	223	GLN
1	A	257	LEU
1	A	302	GLN
1	A	352	ASP
1	D	59	THR
1	D	79	SER
1	D	270	LEU
1	D	352	ASP
1	B	119	ARG
1	B	140	SER
1	B	230	LEU
1	B	259	LEU
1	B	306	THR
1	B	352	ASP

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Mol	Chain	Res	Type
1	C	48	VAL
1	C	182	GLN
1	C	251	GLN
1	C	307	LEU
1	C	352	ASP
1	E	20	SER
1	E	82	ASP
1	E	325	SER
1	F	8	SER
1	F	20	SER
1	F	352	ASP
2	N	543	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	C	251	GLN
1	E	160	ASN
1	F	209	GLN
1	F	251	GLN
1	F	357	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	347/364 (95%)	-0.11	3 (0%) 84 80	21, 41, 80, 100	0
1	B	349/364 (95%)	-0.31	1 (0%) 94 93	17, 35, 63, 93	0
1	C	339/364 (93%)	0.01	6 (1%) 68 61	29, 56, 92, 113	0
1	D	350/364 (96%)	-0.20	1 (0%) 94 93	21, 38, 74, 113	0
1	E	343/364 (94%)	-0.02	2 (0%) 89 86	27, 52, 86, 118	0
1	F	346/364 (95%)	-0.25	0 100 100	21, 37, 62, 110	0
2	I	16/21 (76%)	-0.46	0 100 100	43, 49, 65, 67	0
2	J	16/21 (76%)	-0.29	0 100 100	33, 40, 62, 62	0
2	K	16/21 (76%)	-0.36	0 100 100	26, 35, 54, 60	0
2	L	16/21 (76%)	-0.25	0 100 100	31, 40, 51, 54	0
2	M	16/21 (76%)	-0.35	0 100 100	20, 30, 41, 42	0
2	N	16/21 (76%)	-0.26	0 100 100	28, 34, 48, 51	0
All	All	2170/2310 (93%)	-0.15	13 (0%) 89 86	17, 42, 82, 118	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	TYR	3.3
1	C	164	PRO	3.1
1	E	206	TYR	3.1
1	B	143	THR	2.9
1	C	144	GLY	2.7
1	A	129	THR	2.5
1	C	165	GLU	2.3
1	C	198	SER	2.2
1	D	84	ALA	2.2
1	A	96	GLN	2.2
1	C	199	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	200	GLY	2.1
1	A	161	PHE	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 carbohydrates 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	ZN	C	401	1/1	0.99	0.07	53,53,53,53	0
3	ZN	A	401	1/1	0.99	0.10	39,39,39,39	0
3	ZN	E	401	1/1	1.00	0.08	51,51,51,51	0
3	ZN	D	401	1/1	1.00	0.09	41,41,41,41	0
3	ZN	F	401	1/1	1.00	0.10	39,39,39,39	0
3	ZN	B	401	1/1	1.00	0.09	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.