



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 07:40 AM EDT

PDB ID : 5F5U  
Title : Crystal structure of the Snu23-Prp38-MFAP1(217-258) complex of Chaetomium thermophilum  
Authors : Ulrich, A.K.C.; Seeger, M.; Bartlick, N.; Wahl, M.C.  
Deposited on : 2015-12-04  
Resolution : 2.75 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.37.1
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)	:	2.37.1

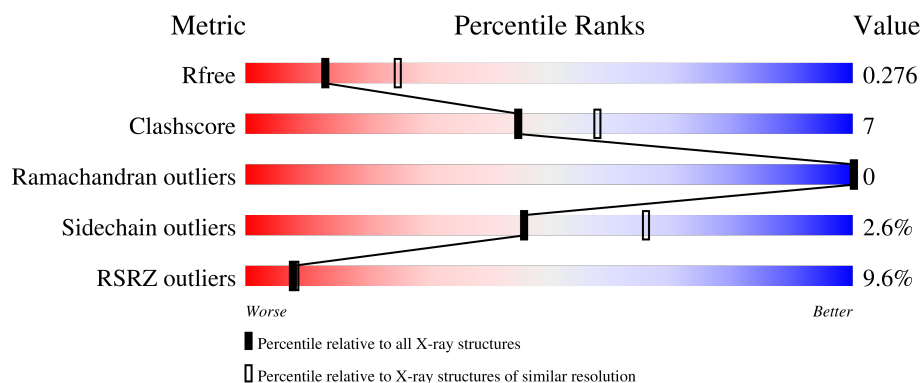
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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  $\geq 3$ , 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	223	<div> <div>3%</div> <div>73%</div> <div>11%</div> <div>16%</div> </div>
1	D	223	<div> <div>9%</div> <div>72%</div> <div>18%</div> <div>9%</div> </div>
1	G	223	<div> <div>10%</div> <div>65%</div> <div>21%</div> <div>13%</div> </div>
2	B	84	<div> <div>5%</div> <div>51%</div> <div>46%</div> </div>
2	E	84	<div> <div>4%</div> <div>38%</div> <div>7%</div> <div>55%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	84	<div><div></div><div>5%</div><div>43%</div><div>7%</div><div>50%</div></div>
3	C	36	<div><div></div><div>14%</div><div>72%</div><div>17%</div><div>11%</div></div>
3	F	36	<div><div></div><div>14%</div><div>58%</div><div>22%</div><div>19%</div></div>
3	I	36	<div><div></div><div>17%</div><div>72%</div><div>6%</div><div>22%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6676 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 Prp38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1530	984	260	280	6			
1	D	202	Total	C	N	O	S	0	0	0
			1636	1044	280	306	6			
1	G	194	Total	C	N	O	S	0	0	0
			1576	1011	268	291	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP G0S1D3
A	-1	ALA	-	expression tag	UNP G0S1D3
A	0	MET	-	expression tag	UNP G0S1D3
A	1	GLY	-	expression tag	UNP G0S1D3
D	-2	GLY	-	expression tag	UNP G0S1D3
D	-1	ALA	-	expression tag	UNP G0S1D3
D	0	MET	-	expression tag	UNP G0S1D3
D	1	GLY	-	expression tag	UNP G0S1D3
G	-2	GLY	-	expression tag	UNP G0S1D3
G	-1	ALA	-	expression tag	UNP G0S1D3
G	0	MET	-	expression tag	UNP G0S1D3
G	1	GLY	-	expression tag	UNP G0S1D3

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	45	Total	C	N	O	S	0	0	0
			374	225	74	74	1			
2	E	38	Total	C	N	O		0	0	0
			334	203	70	61				
2	H	42	Total	C	N	O		0	0	0
			364	219	74	71				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	213	GLY	-	expression tag	UNP G0SHD7
B	214	ALA	-	expression tag	UNP G0SHD7
B	215	MET	-	expression tag	UNP G0SHD7
B	216	GLY	-	expression tag	UNP G0SHD7
E	213	GLY	-	expression tag	UNP G0SHD7
E	214	ALA	-	expression tag	UNP G0SHD7
E	215	MET	-	expression tag	UNP G0SHD7
E	216	GLY	-	expression tag	UNP G0SHD7
H	213	GLY	-	expression tag	UNP G0SHD7
H	214	ALA	-	expression tag	UNP G0SHD7
H	215	MET	-	expression tag	UNP G0SHD7
H	216	GLY	-	expression tag	UNP G0SHD7

- Molecule 3 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	32	Total	C	N	O	0	0	0
			268	168	49	51			
3	F	29	Total	C	N	O	0	0	0
			251	158	46	47			
3	I	28	Total	C	N	O	0	0	0
			242	153	45	44			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	129	GLY	-	expression tag	UNP G0S6R0
C	130	ALA	-	expression tag	UNP G0S6R0
F	129	GLY	-	expression tag	UNP G0S6R0
F	130	ALA	-	expression tag	UNP G0S6R0
I	129	GLY	-	expression tag	UNP G0S6R0
I	130	ALA	-	expression tag	UNP G0S6R0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	7	Total	O	0	0
			7	7		

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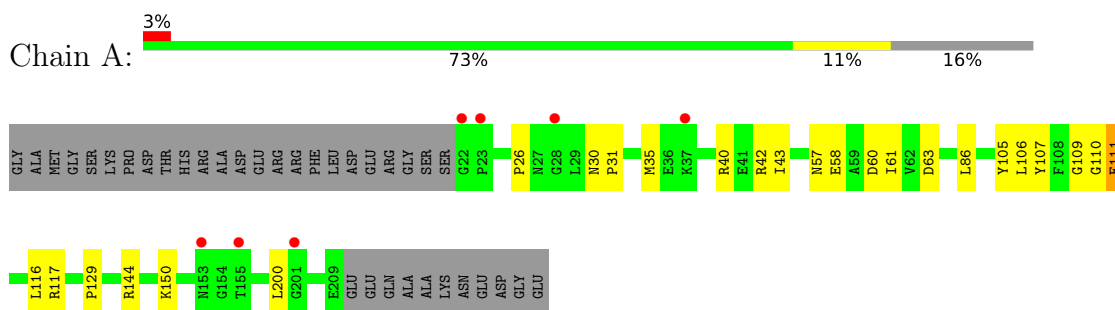
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	5	Total 5	O 5	0	0
4	D	27	Total 27	O 27	0	0
4	E	2	Total 2	O 2	0	0
4	F	3	Total 3	O 3	0	0
4	G	30	Total 30	O 30	0	0
4	H	5	Total 5	O 5	0	0
4	I	2	Total 2	O 2	0	0

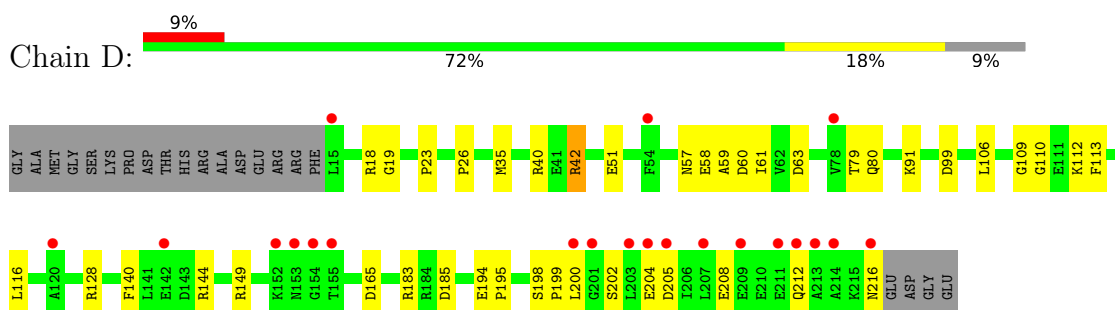
### 3 Residue-property plots [i](#)

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.

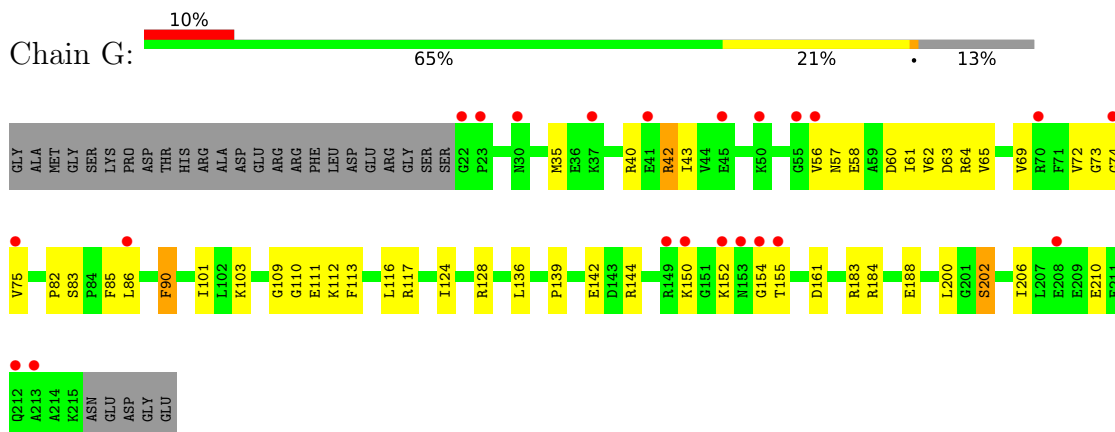
- Molecule 1: Prp38



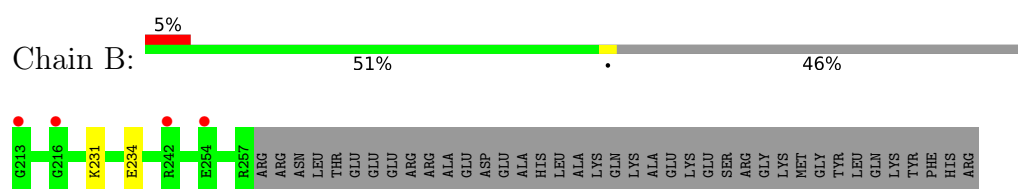
- Molecule 1: Prp38



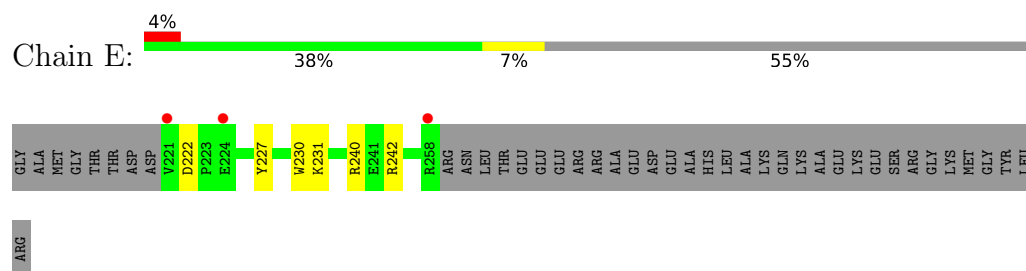
- Molecule 1: Prp38



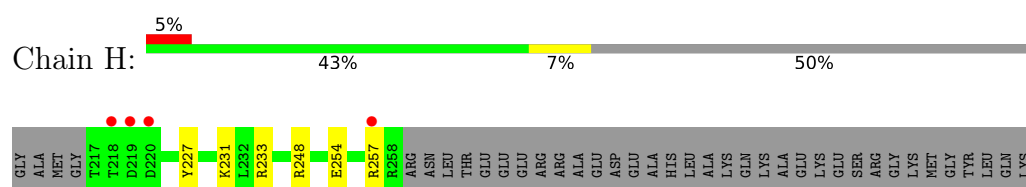
- Molecule 2: Putative uncharacterized protein



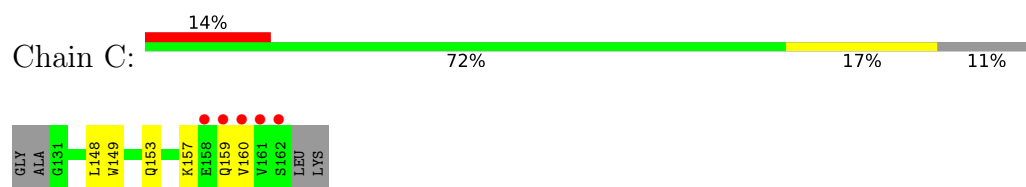
- Molecule 2: Putative uncharacterized protein



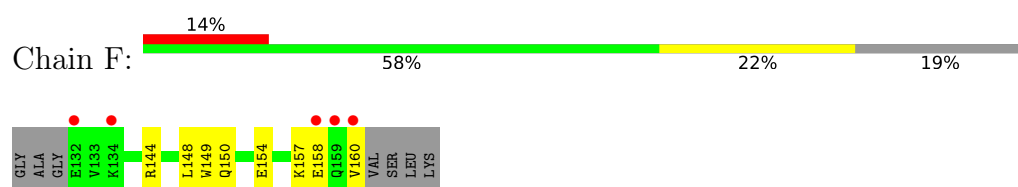
- Molecule 2: Putative uncharacterized protein



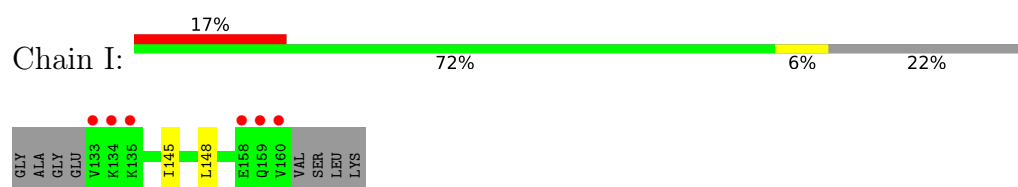
- Molecule 3: Zinc finger domain-containing protein



- Molecule 3: Zinc finger domain-containing protein



- Molecule 3: Zinc finger domain-containing protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.96Å 95.26Å 133.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.75 19.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.93-2.75) 99.8 (19.93-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.75Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.229 , 0.275 0.231 , 0.276	Depositor DCC
$R_{free}$ test set	1527 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 46.2	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	0.94	EDS
Total number of atoms	6676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.63% 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 [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	0.26	0/1561	0.46	0/2107
1	D	0.26	0/1667	0.44	0/2248
1	G	0.26	0/1607	0.45	0/2168
2	B	0.24	0/377	0.44	0/504
2	E	0.23	0/337	0.42	0/449
2	H	0.25	0/367	0.45	0/491
3	C	0.25	0/271	0.37	0/360
3	F	0.26	0/254	0.46	0/337
3	I	0.27	0/245	0.42	0/325
All	All	0.25	0/6686	0.45	0/8989

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	1530	0	1555	16	0
1	D	1636	0	1651	26	0
1	G	1576	0	1598	36	0
2	B	374	0	364	2	0
2	E	334	0	335	5	0
2	H	364	0	357	5	0
3	C	268	0	270	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	251	0	253	6	0
3	I	242	0	247	2	0
4	A	20	0	0	0	0
4	B	7	0	0	0	0
4	C	5	0	0	1	0
4	D	27	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	G	30	0	0	0	0
4	H	5	0	0	0	0
4	I	2	0	0	0	0
All	All	6676	0	6630	86	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 7.

All (86) 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:D:109:GLY:HA3	1:D:116:LEU:HD23	1.76	0.67
1:G:161:ASP:OD2	2:H:233:ARG:NH1	2.27	0.67
1:G:150:LYS:HZ2	1:G:155:THR:HG23	1.60	0.66
1:G:65:VAL:O	1:G:69:VAL:HG22	1.99	0.63
1:G:35:MET:O	1:G:40:ARG:NH1	2.32	0.62
1:G:42:ARG:HD3	1:G:82:PRO:HD3	1.82	0.61
1:G:109:GLY:HA3	1:G:116:LEU:HD23	1.82	0.61
1:D:200:LEU:HD11	2:E:231:LYS:HG2	1.84	0.60
1:D:60:ASP:OD1	3:F:144:ARG:NH1	2.35	0.60
2:H:254:GLU:HG2	2:H:257:ARG:NH2	2.16	0.60
1:A:35:MET:O	1:A:40:ARG:NH1	2.35	0.59
1:G:150:LYS:NZ	1:G:155:THR:HG23	2.18	0.57
3:C:159:GLN:NE2	4:C:201:HOH:O	2.36	0.57
1:G:124:ILE:HD13	1:G:136:LEU:HD13	1.87	0.57
1:A:57:ASN:H	1:A:60:ASP:HB2	1.71	0.56
1:D:200:LEU:O	1:D:204:GLU:HB2	2.06	0.56
1:G:58:GLU:HG2	1:G:101:ILE:HD13	1.86	0.56
1:A:26:PRO:HB2	1:A:129:PRO:HD3	1.89	0.54
2:E:227:TYR:CZ	2:E:231:LYS:HD2	2.42	0.54
1:D:109:GLY:O	1:D:113:PHE:N	2.30	0.53
1:G:62:VAL:HG11	3:I:145:ILE:HG12	1.90	0.52
1:D:165:ASP:OD1	2:E:240:ARG:NH2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:GLY:CA	1:G:117:ARG:HB2	2.40	0.51
1:A:109:GLY:HA3	1:A:116:LEU:HD23	1.93	0.51
1:G:43:ILE:HD11	1:G:86:LEU:HG	1.93	0.50
1:A:105:TYR:O	1:A:110:GLY:N	2.46	0.49
1:G:184:ARG:NH1	1:G:188:GLU:OE2	2.40	0.49
1:D:183:ARG:NH1	1:D:185:ASP:OD2	2.46	0.49
1:G:110:GLY:HA3	1:G:117:ARG:HB2	1.94	0.48
1:D:35:MET:O	1:D:40:ARG:NH1	2.47	0.48
1:G:150:LYS:HG3	1:G:155:THR:HA	1.96	0.48
1:D:194:GLU:HG3	1:D:195:PRO:HD2	1.96	0.48
1:D:112:LYS:HG2	3:F:149:TRP:CD2	2.48	0.48
1:D:59:ALA:HB1	3:F:144:ARG:HD2	1.95	0.47
1:A:107:TYR:O	1:A:111:GLU:HB2	2.14	0.47
1:A:200:LEU:HD21	2:B:231:LYS:HA	1.96	0.47
1:D:57:ASN:H	1:D:60:ASP:HB2	1.79	0.47
1:D:42:ARG:NH1	1:D:80:GLN:O	2.48	0.47
1:G:74:GLY:HA2	1:G:86:LEU:HD22	1.97	0.47
1:G:75:VAL:HA	1:G:82:PRO:HA	1.97	0.47
1:A:58:GLU:O	1:A:61:ILE:HB	2.16	0.46
1:G:57:ASN:H	1:G:60:ASP:HB2	1.80	0.46
3:F:150:GLN:O	3:F:154:GLU:HG2	2.15	0.46
1:G:72:VAL:HG12	1:G:85:PHE:CE1	2.51	0.46
2:H:227:TYR:CE2	2:H:231:LYS:HD2	2.51	0.46
1:G:152:LYS:HA	1:G:152:LYS:HD2	1.69	0.45
1:G:150:LYS:HG2	1:G:154:GLY:O	2.16	0.45
1:G:183:ARG:NH1	2:H:248:ARG:HD3	2.31	0.45
1:D:23:PRO:HB3	1:G:103:LYS:HD3	1.99	0.45
1:D:63:ASP:OD1	3:F:148:LEU:HD11	2.17	0.45
1:D:200:LEU:HD21	1:D:208:GLU:HG2	1.97	0.45
1:A:200:LEU:HD22	2:B:234:GLU:HB3	1.98	0.45
1:A:106:LEU:O	1:A:110:GLY:HA3	2.17	0.45
1:D:58:GLU:O	1:D:61:ILE:HB	2.17	0.45
3:C:149:TRP:O	3:C:153:GLN:HG2	2.17	0.44
1:A:150:LYS:HE2	1:A:150:LYS:HB2	1.81	0.44
1:A:110:GLY:CA	1:A:117:ARG:HB2	2.47	0.44
1:G:56:VAL:HG13	1:G:60:ASP:HB2	2.00	0.43
1:D:19:GLY:HA2	1:G:142:GLU:HG3	2.00	0.43
1:G:200:LEU:HB3	1:G:206:ILE:HG12	2.00	0.43
3:C:157:LYS:HA	3:C:160:VAL:HG22	2.01	0.43
1:D:106:LEU:O	1:D:110:GLY:HA3	2.18	0.43
1:G:57:ASN:O	1:G:61:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:254:GLU:O	2:H:257:ARG:HB2	2.19	0.43
1:G:90:PHE:O	1:G:90:PHE:HD1	2.02	0.43
1:A:43:ILE:HD11	1:A:86:LEU:HG	2.02	0.42
1:D:106:LEU:HD22	1:D:140:PHE:CE2	2.54	0.42
1:D:26:PRO:HG2	1:D:128:ARG:CZ	2.49	0.42
1:G:60:ASP:O	1:G:64:ARG:HG2	2.19	0.42
1:G:109:GLY:O	1:G:113:PHE:N	2.34	0.42
1:G:63:ASP:OD1	3:I:148:LEU:HD11	2.19	0.42
1:D:99:ASP:OD1	1:D:128:ARG:NH2	2.33	0.42
1:G:58:GLU:O	1:G:61:ILE:HB	2.19	0.42
1:A:57:ASN:O	1:A:61:ILE:N	2.49	0.42
1:G:73:GLY:O	1:G:83:SER:OG	2.34	0.42
2:E:242:ARG:HA	2:E:242:ARG:HD2	1.85	0.42
1:A:63:ASP:OD1	3:C:148:LEU:HD11	2.20	0.41
1:G:202:SER:O	1:G:206:ILE:HG13	2.21	0.41
1:D:212:GLN:HE22	1:D:216:ASN:ND2	2.17	0.41
2:E:230:TRP:HE3	2:E:231:LYS:HG3	1.86	0.41
1:G:139:PRO:O	1:G:142:GLU:HG2	2.20	0.41
1:D:202:SER:O	1:D:205:ASP:HB2	2.21	0.41
1:D:198:SER:HA	1:D:199:PRO:HD3	1.80	0.40
3:F:157:LYS:O	3:F:160:VAL:HG22	2.21	0.40
1:D:18:ARG:HD2	1:G:111:GLU:HA	2.04	0.40
1:A:30:ASN:HA	1:A:31:PRO:HD3	1.98	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	186/223 (83%)	186 (100%)	0	0	100	100
1	D	200/223 (90%)	198 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
2	B	43/84 (51%)	43 (100%)	0	0	100	100
2	E	36/84 (43%)	36 (100%)	0	0	100	100
2	H	40/84 (48%)	40 (100%)	0	0	100	100
3	C	30/36 (83%)	30 (100%)	0	0	100	100
3	F	27/36 (75%)	27 (100%)	0	0	100	100
3	I	26/36 (72%)	26 (100%)	0	0	100	100
All	All	780/1029 (76%)	775 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	167/194 (86%)	164 (98%)	3 (2%)	59	75
1	D	178/194 (92%)	172 (97%)	6 (3%)	37	58
1	G	171/194 (88%)	164 (96%)	7 (4%)	30	50
2	B	36/69 (52%)	36 (100%)	0	100	100
2	E	32/69 (46%)	31 (97%)	1 (3%)	40	60
2	H	36/69 (52%)	36 (100%)	0	100	100
3	C	28/30 (93%)	28 (100%)	0	100	100
3	F	26/30 (87%)	25 (96%)	1 (4%)	33	54
3	I	25/30 (83%)	25 (100%)	0	100	100
All	All	699/879 (80%)	681 (97%)	18 (3%)	46	66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG

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Mol	Chain	Res	Type
1	A	111	GLU
1	A	144	ARG
1	D	42	ARG
1	D	51	GLU
1	D	79	THR
1	D	91	LYS
1	D	144	ARG
1	D	149	ARG
2	E	222	ASP
3	F	158	GLU
1	G	42	ARG
1	G	90	PHE
1	G	112	LYS
1	G	128	ARG
1	G	144	ARG
1	G	202	SER
1	G	210	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	212	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 [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	188/223 (84%)	0.03	7 (3%) 41 46	39, 67, 134, 182	0
1	D	202/223 (90%)	0.22	21 (10%) 6 6	43, 70, 193, 251	0
1	G	194/223 (86%)	0.50	22 (11%) 5 5	42, 101, 165, 186	0
2	B	45/84 (53%)	0.37	4 (8%) 9 10	66, 96, 150, 160	0
2	E	38/84 (45%)	0.35	3 (7%) 12 14	76, 98, 151, 178	0
2	H	42/84 (50%)	0.38	4 (9%) 8 8	62, 101, 145, 168	0
3	C	32/36 (88%)	0.78	5 (15%) 2 2	62, 87, 179, 213	0
3	F	29/36 (80%)	1.02	5 (17%) 1 1	74, 109, 175, 217	0
3	I	28/36 (77%)	1.12	6 (21%) 0 0	96, 120, 181, 217	0
All	All	798/1029 (77%)	0.35	77 (9%) 8 8	39, 85, 166, 251	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	155	THR	6.5
3	C	162	SER	6.5
3	I	160	VAL	5.7
3	I	159	GLN	5.6
3	F	160	VAL	5.0
2	H	220	ASP	4.5
1	D	207	LEU	4.4
1	D	203	LEU	4.4
2	H	218	THR	4.3
3	F	132	GLU	4.2
3	F	134	LYS	4.2
3	C	159	GLN	4.0
3	C	160	VAL	3.9
1	G	45	GLU	3.7
1	D	212	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	22	GLY	3.6
3	I	134	LYS	3.6
3	I	133	VAL	3.6
1	A	23	PRO	3.5
3	C	161	VAL	3.5
1	G	22	GLY	3.3
1	G	23	PRO	3.3
1	G	154	GLY	3.3
1	D	155	THR	3.2
2	B	213	GLY	3.1
2	E	221	VAL	3.1
1	G	212	GLN	3.1
1	G	56	VAL	3.1
1	D	154	GLY	3.1
1	G	55	GLY	3.0
1	G	150	LYS	3.0
2	H	219	ASP	3.0
1	G	213	ALA	3.0
1	A	201	GLY	2.9
1	D	204	GLU	2.9
2	B	216	GLY	2.9
3	I	158	GLU	2.9
1	D	216	ASN	2.7
3	F	159	GLN	2.7
1	D	78	VAL	2.7
1	G	153	ASN	2.7
1	G	208	GLU	2.7
1	D	15	LEU	2.6
3	I	135	LYS	2.6
1	D	205	ASP	2.5
3	C	158	GLU	2.5
1	G	75	VAL	2.5
1	G	41	GLU	2.5
1	D	152	LYS	2.4
1	G	74	GLY	2.4
1	A	155	THR	2.4
2	B	254	GLU	2.4
2	E	258	ARG	2.3
1	D	54	PHE	2.3
1	D	213	ALA	2.3
1	D	214	ALA	2.3
1	A	37	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	153	ASN	2.3
1	G	86	LEU	2.3
1	D	211	GLU	2.3
1	G	70	ARG	2.2
1	D	201	GLY	2.2
1	D	209	GLU	2.2
2	H	257	ARG	2.2
1	D	142	GLU	2.2
3	F	158	GLU	2.2
2	E	224	GLU	2.2
1	G	50	LYS	2.1
1	D	120	ALA	2.1
1	A	28	GLY	2.1
1	D	200	LEU	2.1
1	G	149	ARG	2.1
2	B	242	ARG	2.1
1	G	37	LYS	2.1
1	A	153	ASN	2.0
1	G	30	ASN	2.0
1	G	152	LYS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.