



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:53 am BST

PDB ID : 2FW2  
Title : Catalytic domain of CDY  
Authors : Min, J.R.; Antoshenko, T.; Wu, H.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-01-31  
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](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

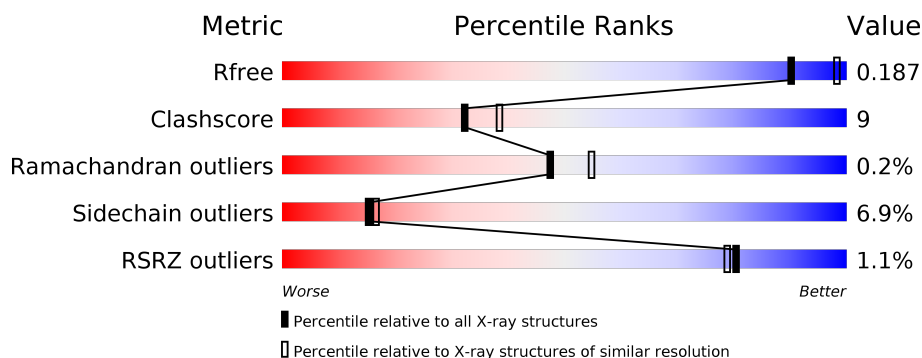
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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 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	260	<div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	B	260	<div> <div>79%</div> <div>15%</div> <div>• •</div> </div>
1	C	260	<div> <div>80%</div> <div>16%</div> <div>• •</div> </div>
1	D	260	<div> <div>%</div> <div>76%</div> <div>20%</div> <div>• •</div> </div>
1	E	260	<div> <div>4%</div> <div>77%</div> <div>19%</div> <div>•</div> </div>
1	F	260	<div> <div>2%</div> <div>76%</div> <div>21%</div> <div>•</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12641 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 Testis-specific chromodomain protein Y 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	2	0
			2018	1281	338	384	15			
1	B	255	Total	C	N	O	S	0	0	0
			1975	1254	332	374	15			
1	C	256	Total	C	N	O	S	0	1	0
			1993	1265	335	378	15			
1	D	257	Total	C	N	O	S	0	0	0
			1989	1263	335	376	15			
1	E	259	Total	C	N	O	S	0	0	0
			1993	1266	335	377	15			
1	F	260	Total	C	N	O	S	0	0	0
			2009	1275	338	381	15			

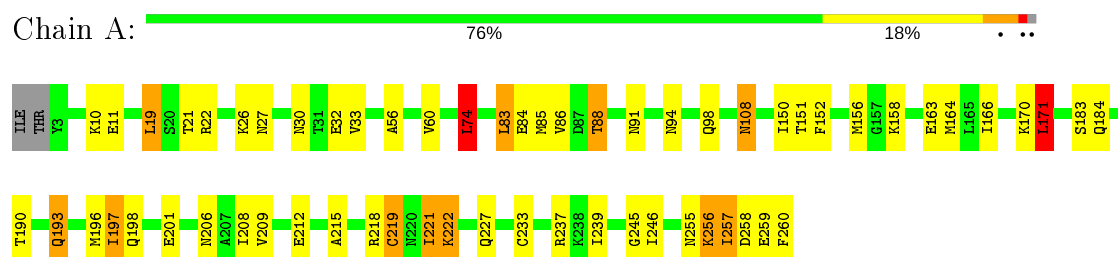
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	152	Total	O	0	0
			152	152		
2	B	123	Total	O	0	0
			123	123		
2	C	134	Total	O	0	0
			134	134		
2	D	101	Total	O	0	0
			101	101		
2	E	70	Total	O	0	0
			70	70		
2	F	84	Total	O	0	0
			84	84		

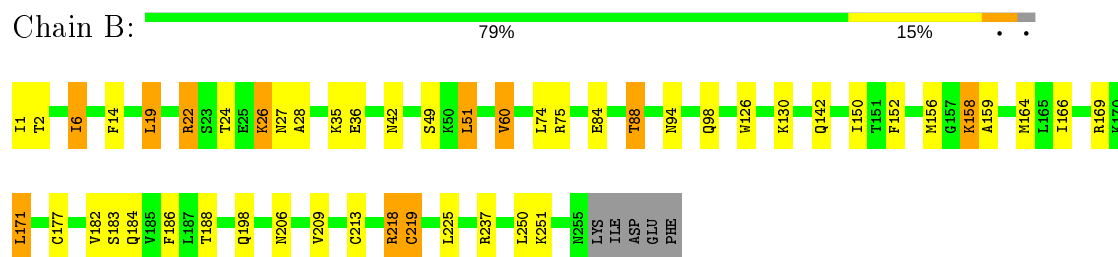
### 3 Residue-property plots [i](#)

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.

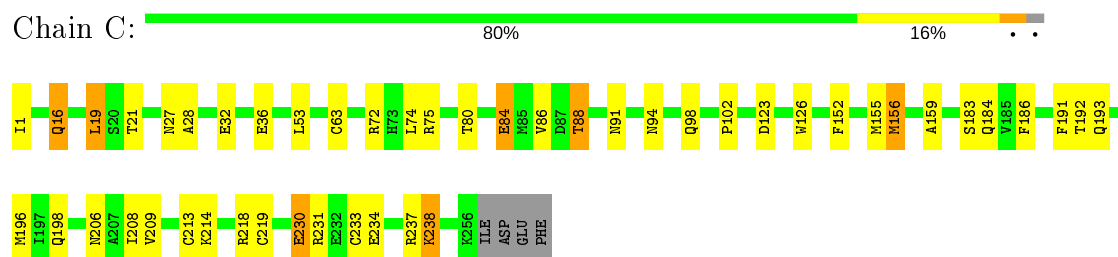
- Molecule 1: Testis-specific chromodomain protein Y 2



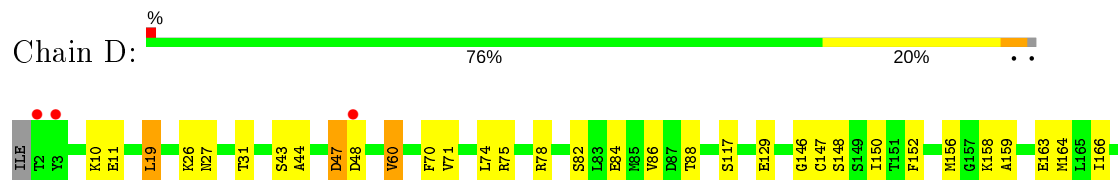
- Molecule 1: Testis-specific chromodomain protein Y 2



- Molecule 1: Testis-specific chromodomain protein Y 2

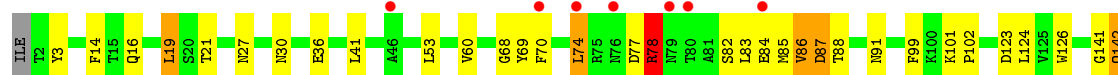
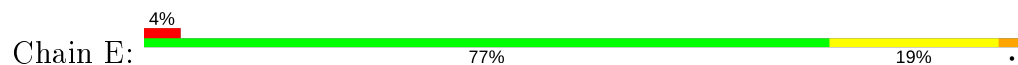


- Molecule 1: Testis-specific chromodomain protein Y 2

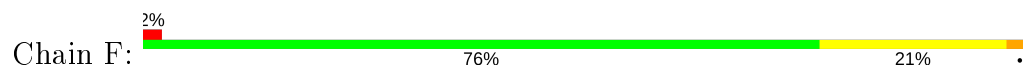




- Molecule 1: Testis-specific chromodomain protein Y 2



- Molecule 1: Testis-specific chromodomain protein Y 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.45Å 133.58Å 82.33Å 90.00° 117.56° 90.00°	Depositor
Resolution (Å)	72.93 – 2.20 48.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (72.93-2.20) 99.3 (48.75-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.253 0.187 , 0.187	Depositor DCC
$R_{free}$ test set	3925 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12641	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

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	0.68	1/2049 (0.0%)	0.75	2/2765 (0.1%)
1	B	0.59	1/2005 (0.0%)	0.72	1/2708 (0.0%)
1	C	0.67	1/2023 (0.0%)	0.69	0/2731
1	D	0.64	2/2019 (0.1%)	0.66	0/2726
1	E	0.68	3/2024 (0.1%)	0.72	2/2733 (0.1%)
1	F	0.56	0/2040	0.65	0/2754
All	All	0.64	8/12160 (0.1%)	0.70	5/16417 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	78	ARG	CZ-NH2	14.43	1.51	1.33
1	E	78	ARG	CZ-NH1	7.91	1.43	1.33
1	C	219	CYS	CB-SG	-7.59	1.69	1.82
1	A	219	CYS	CB-SG	-6.61	1.71	1.82
1	D	213	CYS	CB-SG	-6.07	1.72	1.82
1	B	219	CYS	CB-SG	-5.36	1.73	1.81
1	D	219	CYS	CB-SG	-5.34	1.73	1.81
1	E	78	ARG	CD-NE	5.30	1.55	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	ARG	NE-CZ-NH1	-15.78	112.41	120.30
1	B	51	LEU	CA-CB-CG	6.37	129.95	115.30
1	E	78	ARG	NH1-CZ-NH2	5.37	125.31	119.40
1	A	171	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	74	LEU	CA-CB-CG	5.06	126.94	115.30

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	2018	0	2037	51	0
1	B	1975	0	2010	37	0
1	C	1993	0	2028	31	0
1	D	1989	0	2022	38	0
1	E	1993	0	2007	38	0
1	F	2009	0	2030	48	0
2	A	152	0	0	3	0
2	B	123	0	0	3	0
2	C	134	0	0	4	0
2	D	101	0	0	3	0
2	E	70	0	0	0	0
2	F	84	0	0	5	0
All	All	12641	0	12134	212	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 9.

All (212) 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:C:91:ASN:HB3	2:C:382:HOH:O	1.54	1.04
1:A:257:ILE:HG23	1:A:258:ASP:H	1.18	1.03
1:F:223:LEU:O	1:F:227:GLN:HG3	1.66	0.95
1:A:108:ASN:H	1:A:108:ASN:HD22	1.25	0.84
1:A:257:ILE:CG2	1:A:258:ASP:H	1.89	0.84
1:B:206:ASN:HD22	1:B:209:VAL:H	1.23	0.83
1:B:26:LYS:HD3	1:B:60:VAL:HG11	1.64	0.80
1:E:206:ASN:HD22	1:E:209:VAL:H	1.27	0.79
1:A:257:ILE:HG23	1:A:258:ASP:N	2.00	0.76
1:B:130:LYS:HE3	1:B:188:THR:HG21	1.66	0.76
1:C:94:ASN:HD21	1:C:98:GLN:HE21	1.32	0.75
1:F:31:THR:HG22	1:F:35:LYS:HD2	1.69	0.74
1:A:227:GLN:HE21	1:F:227:GLN:HE22	1.36	0.74
1:D:159:ALA:HB1	1:E:183:SER:HB3	1.69	0.73
1:A:108:ASN:H	1:A:108:ASN:ND2	1.86	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:GLU:O	1:F:88:THR:HG23	1.89	0.72
1:E:142:GLN:HG3	1:E:143:SER:O	1.89	0.72
1:A:206:ASN:HD22	1:A:209:VAL:H	1.37	0.72
1:F:108:ASN:HD22	1:F:108:ASN:H	1.38	0.71
1:F:184:GLN:HG2	1:F:186:PHE:CE2	2.25	0.71
1:D:184:GLN:HE22	1:D:198:GLN:HE22	1.36	0.71
1:D:206:ASN:HD22	1:D:209:VAL:H	1.37	0.71
1:B:84:GLU:O	1:B:88:THR:HG23	1.91	0.69
1:B:6:ILE:HD11	1:B:36:GLU:HB3	1.75	0.68
1:C:206:ASN:HD22	1:C:209:VAL:H	1.41	0.68
1:B:94:ASN:HD21	1:B:98:GLN:HE21	1.41	0.68
1:F:74:LEU:HB3	1:F:246:ILE:CD1	2.23	0.68
1:F:108:ASN:H	1:F:108:ASN:ND2	1.91	0.67
1:C:184:GLN:HE22	1:C:198:GLN:HE22	1.42	0.67
1:A:257:ILE:CG2	1:A:258:ASP:N	2.54	0.67
1:A:163:GLU:CG	1:B:183:SER:HB2	2.25	0.67
1:F:4:ARG:HG3	2:F:281:HOH:O	1.95	0.65
1:D:71:VAL:O	1:D:75:ARG:HG3	1.96	0.65
1:F:19:LEU:HD13	1:F:27:ASN:HB3	1.77	0.65
1:B:126:TRP:HB3	1:B:186:PHE:CE2	2.32	0.65
1:F:194:GLU:HG2	2:F:292:HOH:O	1.97	0.64
1:E:231:ARG:HD3	1:F:219:CYS:SG	2.39	0.62
1:A:184:GLN:HE22	1:A:198:GLN:HE22	1.47	0.62
1:F:206:ASN:HD22	1:F:209:VAL:H	1.45	0.62
1:A:190:THR:HB	1:A:193:GLN:HG2	1.82	0.62
1:F:244:GLN:HG2	2:F:335:HOH:O	2.00	0.61
1:C:84[A]:GLU:O	1:C:88:THR:HG23	2.01	0.61
1:C:231:ARG:NH1	2:C:288:HOH:O	2.33	0.61
1:C:126:TRP:HB3	1:C:186:PHE:CE2	2.36	0.60
1:E:253:VAL:O	1:E:254:GLU:HB2	2.00	0.60
1:A:91:ASN:HB3	2:A:404:HOH:O	2.02	0.60
1:D:150:ILE:HD11	1:D:225:LEU:HD23	1.83	0.60
1:B:164:MET:SD	1:B:171:LEU:HD22	2.42	0.59
1:B:159:ALA:HB1	1:C:183:SER:HB3	1.86	0.58
1:B:19:LEU:HD13	1:B:27:ASN:HB3	1.86	0.58
1:E:150:ILE:HD11	1:E:225:LEU:HD23	1.86	0.58
1:A:218:ARG:NH2	1:A:222:LYS:HE3	2.19	0.57
1:E:152:PHE:O	1:E:156:MET:HG2	2.04	0.57
1:D:74:LEU:HD11	1:D:82:SER:HB3	1.86	0.57
1:F:117:SER:HB2	1:F:148:SER:HB3	1.87	0.57
1:F:75:ARG:HE	1:F:250:LEU:HD21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:NZ	1:B:218:ARG:NH2	2.53	0.57
1:F:43:SER:HB2	2:F:280:HOH:O	2.05	0.57
1:A:19:LEU:HD13	1:A:27:ASN:HB3	1.87	0.56
1:B:166:ILE:HD11	1:C:213:CYS:HB2	1.88	0.56
1:F:24:THR:HB	1:F:28:ALA:HB3	1.87	0.56
1:A:255:ASN:O	1:A:256:LYS:O	2.23	0.56
1:B:206:ASN:ND2	1:B:209:VAL:H	1.98	0.55
1:D:183:SER:HB2	1:F:163:GLU:CG	2.37	0.55
1:E:206:ASN:HB3	1:E:209:VAL:HB	1.89	0.55
1:F:256:LYS:HD3	2:F:341:HOH:O	2.05	0.55
1:C:21:THR:H	1:C:27:ASN:ND2	2.03	0.55
1:D:146:GLY:O	1:D:147:CYS:HB2	2.06	0.55
1:F:94:ASN:HD21	1:F:98:GLN:HE21	1.54	0.55
1:A:166:ILE:HD11	1:B:213:CYS:HB2	1.89	0.54
1:B:158:LYS:HE2	1:C:218:ARG:NH1	2.21	0.54
1:A:163:GLU:HG2	1:B:183:SER:HB2	1.90	0.54
1:D:240:TRP:O	1:D:246:ILE:HD11	2.08	0.54
1:E:102:PRO:HA	1:E:123:ASP:OD2	2.07	0.54
1:D:84:GLU:O	1:D:88:THR:HG23	2.08	0.54
1:C:19:LEU:HD13	1:C:27:ASN:HB3	1.90	0.54
1:F:53:LEU:HD11	1:F:106:SER:HB2	1.90	0.53
1:C:230:GLU:HG2	1:C:234:GLU:OE2	2.08	0.53
1:E:83:LEU:O	1:E:87:ASP:HB2	2.07	0.53
1:B:184:GLN:HE22	1:B:198:GLN:HE22	1.56	0.53
1:D:166:ILE:HD11	1:E:213:CYS:HB3	1.90	0.53
1:A:227:GLN:HE21	1:F:227:GLN:NE2	2.06	0.53
1:E:184:GLN:HE22	1:E:198:GLN:HE22	1.57	0.53
1:D:19:LEU:HD13	1:D:27:ASN:HB3	1.91	0.53
1:F:184:GLN:HE22	1:F:198:GLN:HE22	1.55	0.53
1:A:215:ALA:O	1:A:219:CYS:HB2	2.09	0.53
1:D:258:ASP:CB	2:D:337:HOH:O	2.55	0.52
1:D:86:VAL:HG13	1:D:233:CYS:HB3	1.90	0.52
1:E:186:PHE:HB2	1:E:191:PHE:HD1	1.74	0.52
1:A:56:ALA:HB3	1:A:108:ASN:HD21	1.75	0.52
1:F:71:VAL:O	1:F:75:ARG:HB2	2.10	0.52
1:A:30:ASN:OD1	1:A:33:VAL:HG23	2.10	0.52
1:A:26:LYS:HD2	1:A:260:PHE:CD1	2.45	0.52
1:A:84:GLU:O	1:A:88:THR:HG23	2.10	0.52
1:A:197:ILE:O	1:A:201:GLU:HG3	2.10	0.52
1:F:74:LEU:HB3	1:F:246:ILE:HD12	1.92	0.52
1:A:21:THR:H	1:A:27:ASN:ND2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LYS:HZ1	1:E:221:ILE:HD11	1.75	0.51
1:F:56:ALA:HB3	1:F:108:ASN:HD21	1.76	0.51
1:C:152:PHE:O	1:C:156:MET:HG3	2.09	0.51
1:E:68:GLY:HA2	1:E:253:VAL:HG21	1.91	0.51
1:F:6:ILE:HD11	1:F:40:ALA:HB2	1.92	0.51
1:A:98:GLN:OE1	1:A:222:LYS:HE2	2.09	0.51
1:C:186:PHE:HB2	1:C:191:PHE:HD1	1.76	0.51
1:E:14:PHE:HE1	1:E:16:GLN:HG3	1.76	0.51
1:D:183:SER:HB2	1:F:163:GLU:HG2	1.92	0.51
1:D:196:MET:O	1:D:200:LYS:HE3	2.11	0.50
1:B:24:THR:HB	1:B:28:ALA:HB3	1.94	0.50
1:C:28:ALA:HB2	1:C:63:CYS:SG	2.51	0.50
1:A:221:ILE:HD12	2:A:301:HOH:O	2.12	0.49
1:A:94:ASN:HD21	1:A:98:GLN:HE21	1.60	0.49
1:D:215:ALA:HA	1:D:218:ARG:HD3	1.95	0.49
1:F:94:ASN:ND2	1:F:98:GLN:HE21	2.11	0.49
1:A:152:PHE:O	1:A:156:MET:HG2	2.12	0.49
1:E:19:LEU:HD13	1:E:27:ASN:HB3	1.94	0.49
1:D:174:ARG:HG2	1:D:174:ARG:HH11	1.78	0.49
1:A:166:ILE:HD11	1:B:213:CYS:CB	2.43	0.48
1:D:242:SER:O	1:D:246:ILE:HG12	2.13	0.48
1:B:130:LYS:HG2	1:B:188:THR:CG2	2.43	0.48
1:A:83:LEU:HB3	1:F:83:LEU:HG	1.94	0.48
1:D:164:MET:SD	1:D:171:LEU:HD22	2.54	0.48
1:D:74:LEU:HB3	1:D:246:ILE:HD12	1.96	0.47
1:D:163:GLU:OE2	1:E:124:LEU:HD22	2.14	0.47
1:D:221:ILE:O	1:D:221:ILE:HG13	2.13	0.47
1:D:152:PHE:O	1:D:156:MET:HG2	2.13	0.47
1:E:152:PHE:HB2	1:E:153:PRO:HD3	1.95	0.47
1:A:239:ILE:O	1:A:245:GLY:HA3	2.14	0.47
1:C:155:MET:HG3	1:C:156:MET:HG2	1.95	0.47
1:A:86:VAL:HG13	1:A:233:CYS:HB3	1.96	0.47
1:C:88:THR:HG22	2:C:392:HOH:O	2.15	0.47
1:D:70:PHE:HD2	2:D:353:HOH:O	1.98	0.47
1:E:21:THR:H	1:E:27:ASN:ND2	2.13	0.46
1:F:152:PHE:O	1:F:156:MET:HG2	2.15	0.46
1:C:94:ASN:ND2	1:C:98:GLN:HE21	2.07	0.46
1:E:30:ASN:HB2	1:E:69:TYR:CD1	2.51	0.46
1:B:150:ILE:HD11	1:B:225:LEU:HD23	1.97	0.46
1:D:257:ILE:H	1:D:257:ILE:HD13	1.81	0.46
1:E:74:LEU:HD21	1:E:85:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:ASN:HD22	1:F:209:VAL:HG23	1.81	0.46
1:A:158:LYS:HZ3	1:B:218:ARG:HH21	1.63	0.46
1:C:75:ARG:HD3	2:C:338:HOH:O	2.15	0.46
1:D:163:GLU:HG2	1:E:183:SER:HB2	1.98	0.45
1:B:142:GLN:HB3	2:B:307:HOH:O	2.15	0.45
1:C:192:THR:O	1:C:196:MET:HG2	2.16	0.45
1:A:212:GLU:OE2	1:C:238:LYS:NZ	2.49	0.45
1:A:219:CYS:SG	1:C:231:ARG:HD3	2.56	0.45
1:A:158:LYS:HZ3	1:B:218:ARG:NH2	2.14	0.45
1:B:94:ASN:ND2	1:B:98:GLN:HE21	2.11	0.45
1:D:188:THR:CG2	2:D:355:HOH:O	2.64	0.45
1:F:177:CYS:HA	1:F:182:VAL:O	2.17	0.45
1:F:74:LEU:HD23	1:F:246:ILE:HD13	1.99	0.45
1:E:82:SER:O	1:E:86:VAL:HB	2.17	0.45
1:D:117:SER:HB2	1:D:148:SER:HB3	1.99	0.44
1:F:214:LYS:O	1:F:218:ARG:HB3	2.17	0.44
1:B:14:PHE:HA	1:B:49:SER:HB2	2.00	0.44
1:D:220:ASN:HD21	1:F:154:LYS:HE2	1.83	0.44
1:B:22:ARG:NH2	2:B:378:HOH:O	2.50	0.44
1:C:32:GLU:O	1:C:36:GLU:HG3	2.17	0.44
1:F:81:ALA:O	1:F:85:MET:HB2	2.18	0.44
1:B:130:LYS:HE3	1:B:188:THR:CG2	2.43	0.44
1:A:74:LEU:HB3	1:A:246:ILE:CD1	2.48	0.44
1:A:163:GLU:HG3	1:B:183:SER:HB2	1.99	0.43
1:E:141:GLY:HA3	1:E:248:SER:HB3	2.00	0.43
1:D:158:LYS:NZ	1:E:221:ILE:HD11	2.32	0.43
1:E:70:PHE:O	1:E:74:LEU:HD22	2.17	0.43
1:F:26:LYS:HB2	1:F:60:VAL:HG22	1.99	0.43
1:C:102:PRO:HA	1:C:123:ASP:OD2	2.17	0.43
1:D:206:ASN:HD21	1:D:208:ILE:HB	1.84	0.43
1:E:196:MET:O	1:E:199:ILE:HG22	2.19	0.43
1:A:74:LEU:HD21	1:A:85:MET:SD	2.59	0.43
1:F:4:ARG:O	1:F:22:ARG:HD3	2.18	0.43
1:B:42:ASN:ND2	2:B:329:HOH:O	2.43	0.43
1:A:10[A]:LYS:HE3	1:A:10[A]:LYS:HB3	1.66	0.43
1:A:197:ILE:HG21	1:A:197:ILE:HD12	1.73	0.43
1:E:77:ASP:O	1:E:78:ARG:C	2.57	0.43
1:B:206:ASN:ND2	1:B:209:VAL:HG23	2.33	0.43
1:F:184:GLN:NE2	1:F:198:GLN:HE22	2.17	0.42
1:C:86:VAL:HG13	1:C:233:CYS:HB3	2.01	0.42
1:E:206:ASN:ND2	1:E:209:VAL:H	2.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ALA:HA	1:D:47:ASP:OD2	2.20	0.42
1:D:129:GLU:OE2	1:D:188:THR:HG22	2.19	0.42
1:E:84:GLU:O	1:E:88:THR:HG22	2.20	0.42
1:F:5:ASP:OD2	1:F:36:GLU:OE2	2.38	0.42
1:B:6:ILE:HG22	1:B:19:LEU:HA	2.01	0.42
1:D:159:ALA:CB	1:E:183:SER:HB3	2.44	0.42
1:B:166:ILE:HD11	1:C:213:CYS:CB	2.49	0.42
1:E:53:LEU:HD13	1:E:199:ILE:HD13	2.01	0.42
1:E:30:ASN:HB2	1:E:69:TYR:CE1	2.55	0.42
1:C:84[B]:GLU:O	1:C:88:THR:HG23	2.20	0.41
1:A:227:GLN:HG2	1:F:227:GLN:NE2	2.35	0.41
1:F:150:ILE:O	1:F:154:LYS:HD2	2.20	0.41
1:A:183:SER:HB3	1:C:159:ALA:HB1	2.02	0.41
1:B:177:CYS:HA	1:B:182:VAL:O	2.21	0.41
1:A:193:GLN:H	1:A:193:GLN:CD	2.24	0.41
1:A:170:LYS:HZ1	1:A:259:GLU:CD	2.24	0.41
1:E:163:GLU:HG2	1:F:183:SER:HB2	2.01	0.41
1:E:41:LEU:O	1:E:99:PHE:HE1	2.03	0.41
1:A:150:ILE:HG13	1:A:151:THR:N	2.35	0.41
1:B:152:PHE:O	1:B:156:MET:HG2	2.20	0.41
1:F:237:ARG:HG3	1:F:238:LYS:N	2.35	0.41
1:D:26:LYS:HB3	1:D:60:VAL:HG11	2.02	0.41
1:A:164:MET:SD	1:A:171:LEU:HD22	2.61	0.41
1:D:252:TYR:O	1:D:256:LYS:HB3	2.20	0.41
1:E:3:TYR:HB3	1:E:36:GLU:OE2	2.21	0.41
1:F:94:ASN:O	1:F:98:GLN:HG2	2.21	0.41
1:C:206:ASN:HD21	1:C:208:ILE:HB	1.85	0.41
1:A:206:ASN:HD21	1:A:208:ILE:HB	1.86	0.40
1:F:155:MET:HG3	1:F:179:LYS:O	2.21	0.40
1:B:130:LYS:CG	1:B:188:THR:CG2	3.00	0.40
1:A:32:GLU:HB2	2:A:385:HOH:O	2.21	0.40
1:C:16:GLN:HG2	1:C:53:LEU:HD23	2.04	0.40
1:E:126:TRP:HB3	1:E:186:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

## 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	258/260 (99%)	251 (97%)	6 (2%)	1 (0%)	34	37
1	B	253/260 (97%)	248 (98%)	5 (2%)	0	100	100
1	C	255/260 (98%)	250 (98%)	5 (2%)	0	100	100
1	D	255/260 (98%)	250 (98%)	5 (2%)	0	100	100
1	E	257/260 (99%)	247 (96%)	8 (3%)	2 (1%)	19	19
1	F	258/260 (99%)	253 (98%)	5 (2%)	0	100	100
All	All	1536/1560 (98%)	1499 (98%)	34 (2%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	LYS
1	E	254	GLU
1	E	78	ARG

### 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	222/223 (100%)	206 (93%)	16 (7%)	14	15
1	B	218/223 (98%)	198 (91%)	20 (9%)	9	9
1	C	220/223 (99%)	205 (93%)	15 (7%)	16	17
1	D	219/223 (98%)	205 (94%)	14 (6%)	17	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	217/223 (97%)	205 (94%)	12 (6%)	21	26
1	F	220/223 (99%)	206 (94%)	14 (6%)	17	20
All	All	1316/1338 (98%)	1225 (93%)	91 (7%)	15	16

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	19	LEU
1	A	22	ARG
1	A	60	VAL
1	A	74	LEU
1	A	83	LEU
1	A	88	THR
1	A	108	ASN
1	A	171	LEU
1	A	193	GLN
1	A	196	MET
1	A	197	ILE
1	A	221	ILE
1	A	222	LYS
1	A	237	ARG
1	A	257	ILE
1	B	1	ILE
1	B	2	THR
1	B	6	ILE
1	B	19	LEU
1	B	22	ARG
1	B	26	LYS
1	B	35	LYS
1	B	51	LEU
1	B	60	VAL
1	B	74	LEU
1	B	75	ARG
1	B	88	THR
1	B	158	LYS
1	B	169	ARG
1	B	171	LEU
1	B	218	ARG
1	B	219	CYS
1	B	237	ARG

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Mol	Chain	Res	Type
1	B	250	LEU
1	B	251	LYS
1	C	1	ILE
1	C	16	GLN
1	C	19	LEU
1	C	72	ARG
1	C	74	LEU
1	C	80	THR
1	C	84[A]	GLU
1	C	84[B]	GLU
1	C	88	THR
1	C	156	MET
1	C	193	GLN
1	C	214	LYS
1	C	230	GLU
1	C	237	ARG
1	C	238	LYS
1	D	10	LYS
1	D	11	GLU
1	D	19	LEU
1	D	31	THR
1	D	43	SER
1	D	47	ASP
1	D	48	ASP
1	D	60	VAL
1	D	78	ARG
1	D	171	LEU
1	D	192	THR
1	D	220	ASN
1	D	221	ILE
1	D	257	ILE
1	E	19	LEU
1	E	60	VAL
1	E	74	LEU
1	E	86	VAL
1	E	87	ASP
1	E	91	ASN
1	E	101	LYS
1	E	142	GLN
1	E	192	THR
1	E	193	GLN
1	E	237	ARG

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Mol	Chain	Res	Type
1	E	253	VAL
1	F	6	ILE
1	F	16	GLN
1	F	19	LEU
1	F	60	VAL
1	F	83	LEU
1	F	88	THR
1	F	108	ASN
1	F	155	MET
1	F	171	LEU
1	F	193	GLN
1	F	196	MET
1	F	218	ARG
1	F	237	ARG
1	F	251	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	42	ASN
1	A	94	ASN
1	A	108	ASN
1	A	162	ASN
1	A	184	GLN
1	A	206	ASN
1	A	244	GLN
1	B	27	ASN
1	B	42	ASN
1	B	73	HIS
1	B	94	ASN
1	B	198	GLN
1	B	206	ASN
1	C	27	ASN
1	C	39	ASN
1	C	94	ASN
1	C	162	ASN
1	C	193	GLN
1	C	198	GLN
1	C	206	ASN
1	C	220	ASN
1	C	244	GLN

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Mol	Chain	Res	Type
1	D	16	GLN
1	D	27	ASN
1	D	39	ASN
1	D	42	ASN
1	D	73	HIS
1	D	162	ASN
1	D	184	GLN
1	D	193	GLN
1	D	206	ASN
1	E	27	ASN
1	E	42	ASN
1	E	94	ASN
1	E	198	GLN
1	E	206	ASN
1	E	244	GLN
1	F	27	ASN
1	F	39	ASN
1	F	42	ASN
1	F	94	ASN
1	F	108	ASN
1	F	162	ASN
1	F	184	GLN
1	F	206	ASN
1	F	227	GLN
1	F	244	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](#)

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	258/260 (99%)	-0.11	0	100 100	15, 22, 35, 50	0
1	B	255/260 (98%)	-0.24	0	100 100	20, 27, 40, 47	0
1	C	256/260 (98%)	-0.31	0	100 100	18, 26, 34, 41	0
1	D	257/260 (98%)	-0.10	3 (1%)	79 77	19, 29, 41, 50	0
1	E	259/260 (99%)	0.10	10 (3%)	39 37	24, 37, 56, 61	0
1	F	260/260 (100%)	-0.04	4 (1%)	73 72	21, 33, 45, 49	0
All	All	1545/1560 (99%)	-0.12	17 (1%)	80 79	15, 28, 45, 61	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	250	LEU	3.7
1	E	70	PHE	3.2
1	E	74	LEU	3.2
1	D	2	THR	3.0
1	E	253	VAL	3.0
1	E	84	GLU	2.8
1	F	211	GLU	2.8
1	E	246	ILE	2.8
1	E	79	ASN	2.5
1	E	76	ASN	2.4
1	D	48	ASP	2.4
1	E	80	THR	2.3
1	D	3	TYR	2.3
1	E	46	ALA	2.2
1	F	22	ARG	2.2
1	F	76	ASN	2.2
1	F	4	ARG	2.1

## 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.