WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 04:33 AM EDT

PDB ID	:	7LW2
Title	:	Crystal structure of EV-D68 2A protease N84T mutant
Authors	:	Liu, C.; Lee, M.-Y.; Liu, W.; Wang, J.
Deposited on	:	2021-02-27
Resolution	:	2.57 Å(reported)

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

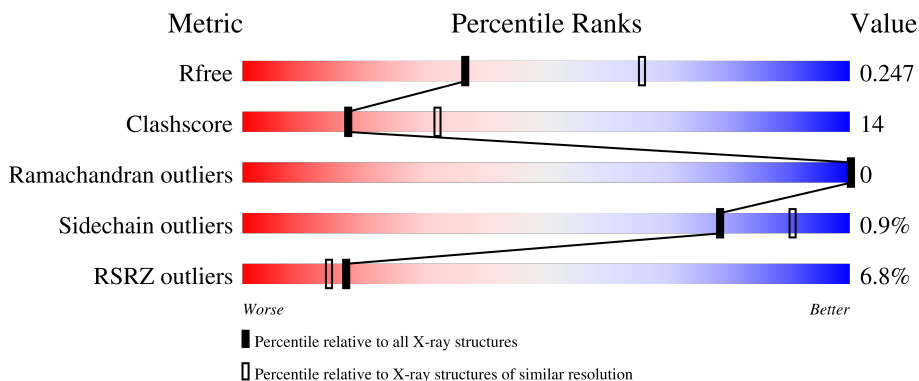|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.57 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		14
Ramachandran outliers		0
Sidechain outliers		0.9%
RSRZ outliers		6.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	147	9% 73% 23% • •
1	B	147	5% 74% 22% •
1	C	147	7% 72% 24% •
1	D	147	7% 75% 21% • •
1	E	147	3% 79% 18% •

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Mol	Chain	Length	Quality of chain
1	F	147	

8%

73%

24%

2　Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11430 atoms, of which 5261 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 Protease 2A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	142	Total	C	H	N	O	S	0	0	0
			1967	658	931	182	190	6			
1	A	142	Total	C	H	N	O	S	0	0	0
			1900	647	882	178	187	6			
1	B	142	Total	C	H	N	O	S	0	0	0
			1935	658	900	182	189	6			
1	C	141	Total	C	H	N	O	S	0	0	0
			1838	633	834	178	187	6			
1	D	142	Total	C	H	N	O	S	0	0	0
			1907	646	888	178	189	6			
1	F	142	Total	C	H	N	O	S	0	0	0
			1842	645	826	177	188	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	84	THR	ASN	engineered mutation	UNP A0A097BW19
A	84	THR	ASN	engineered mutation	UNP A0A097BW19
B	84	THR	ASN	engineered mutation	UNP A0A097BW19
C	84	THR	ASN	engineered mutation	UNP A0A097BW19
D	84	THR	ASN	engineered mutation	UNP A0A097BW19
F	84	THR	ASN	engineered mutation	UNP A0A097BW19

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

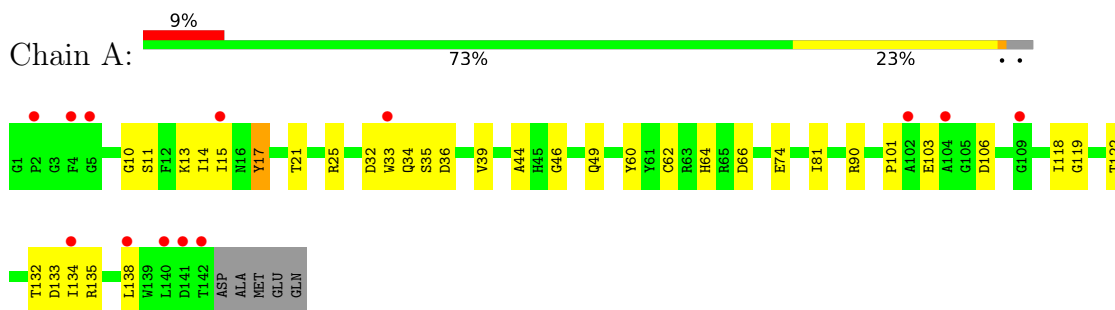| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	10	Total 10	O 10	0	0
3	A	8	Total 8	O 8	0	0
3	B	10	Total 10	O 10	0	0
3	D	5	Total 5	O 5	0	0
3	F	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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.
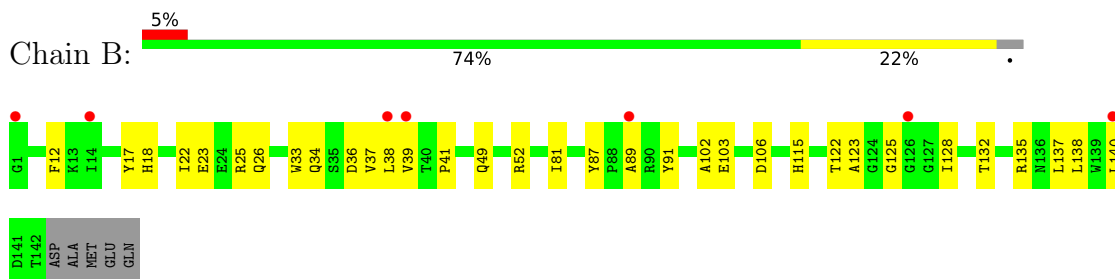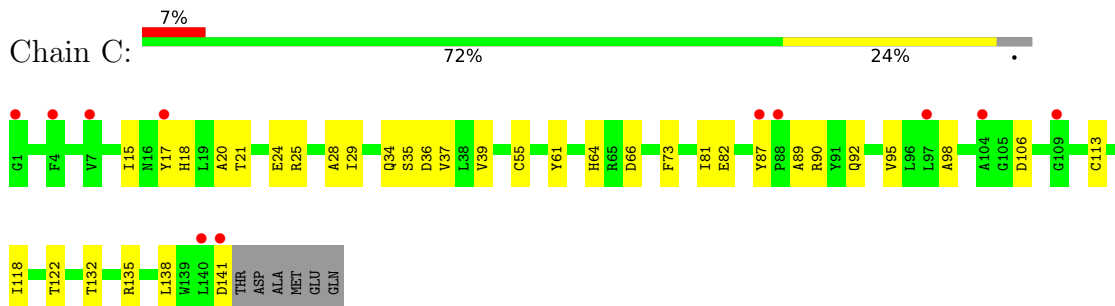
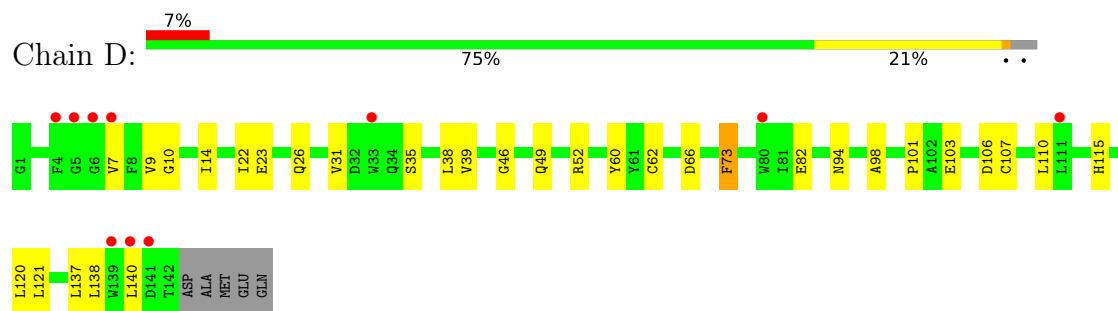- Molecule 1: Protease 2A
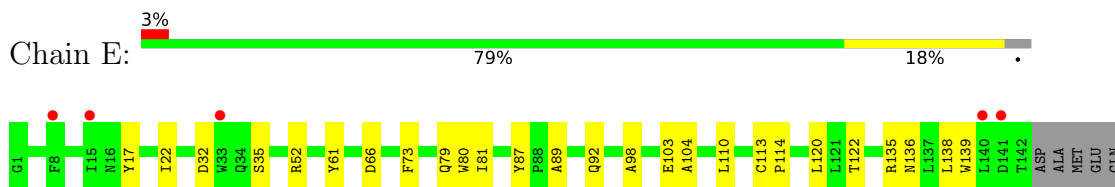
Chain E:

- Molecule 1: Protease 2A

Chain A:

- Molecule 1: Protease 2A

Chain B:

- Molecule 1: Protease 2A

Chain C:

• Molecule 1: Protease 2A

Chain D:

• Molecule 1: Protease 2A

Chain F:
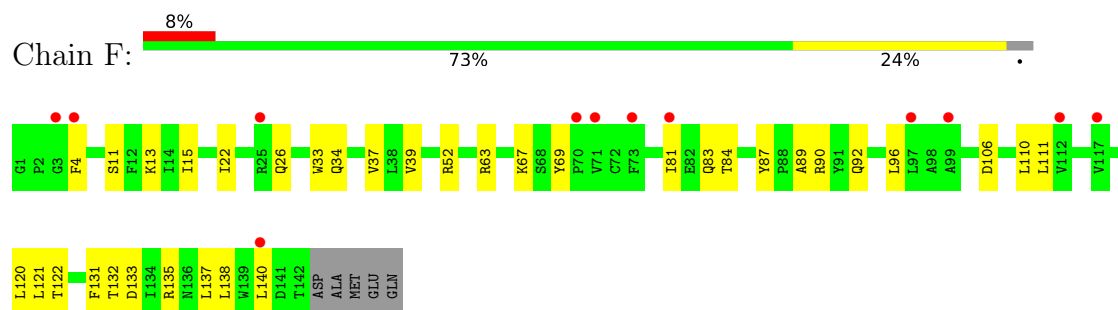
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	119.25Å 119.25Å 80.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.43 – 2.57 44.43 – 2.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.43-2.57) 99.9 (44.43-2.57)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.58Å)	Xtriage
Refinement program	PHENIX dev_3893	Depositor
R, R_{free}	0.215 , 0.242 0.220 , 0.247	Depositor DCC
R_{free} test set	1984 reflections (5.49%)	wwPDB-VP
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 65.9	EDS
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11430	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.41	0/1044	0.56	0/1425
1	B	0.28	0/1061	0.55	0/1446
1	C	0.32	0/1030	0.57	0/1403
1	D	0.48	0/1045	0.56	0/1427
1	E	0.31	0/1062	0.50	0/1448
1	F	0.40	0/1042	0.60	0/1420
All	All	0.37	0/6284	0.56	0/8569

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 ⓘ

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	1018	882	932	31	0
1	B	1035	900	967	31	0
1	C	1004	834	881	28	0
1	D	1019	888	924	22	0
1	E	1036	931	967	20	0
1	F	1016	826	914	38	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	8	0	0	0	0
3	B	10	0	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	F	2	0	0	0	0
All	All	6169	5261	5585	162	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 14.

All (162) 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:F:96:LEU:HD11	1:F:133:ASP:HB2	1.37	1.06
1:B:22:ILE:HG13	1:B:23:GLU:N	1.72	1.05
1:F:83:GLN:NE2	1:F:84:THR:O	1.98	0.96
1:B:22:ILE:HG13	1:B:23:GLU:H	1.31	0.95
1:B:37:VAL:HG11	1:B:132:THR:HG21	1.47	0.94
1:B:37:VAL:CG1	1:B:132:THR:HG21	2.02	0.89
1:B:52:ARG:HG2	1:B:138:LEU:HD13	1.54	0.89
1:E:61:TYR:OH	1:E:66:ASP:OD1	1.91	0.88
1:A:14:ILE:HG12	1:A:39:VAL:HG22	1.56	0.86
1:A:74:GLU:HG3	1:F:81:ILE:HB	1.58	0.85
1:E:52:ARG:HG2	1:E:138:LEU:HD23	1.57	0.84
1:C:21:THR:HG23	1:C:24:GLU:OE2	1.76	0.84
1:B:52:ARG:CG	1:B:138:LEU:HD13	2.10	0.82
1:F:137:LEU:HD22	1:F:140:LEU:HD21	1.62	0.81
1:F:37:VAL:CG1	1:F:132:THR:HG21	2.14	0.78
1:E:139:TRP:CE3	1:A:34:GLN:NE2	2.53	0.76
1:D:73:PHE:HB3	1:D:98:ALA:HB2	1.69	0.75
1:F:96:LEU:HD11	1:F:133:ASP:CB	2.16	0.75
1:F:137:LEU:O	1:F:140:LEU:HD23	1.88	0.74
1:E:52:ARG:CG	1:E:138:LEU:HD23	2.18	0.73
1:F:67:LYS:HD3	1:F:69:TYR:CE1	2.25	0.71
1:E:103:GLU:HG3	1:E:104:ALA:H	1.56	0.71
1:C:25:ARG:NH2	1:F:26:GLN:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:LEU:HD13	1:F:131:PHE:CE2	2.26	0.70
1:C:61:TYR:OH	1:C:66:ASP:OD1	2.09	0.69
1:F:52:ARG:O	1:F:52:ARG:HD2	1.94	0.68
1:A:81:ILE:HA	1:A:90:ARG:O	1.94	0.68
1:A:81:ILE:HG22	1:C:141:ASP:O	1.94	0.66
1:C:81:ILE:CG2	1:C:89:ALA:HB1	2.26	0.66
1:B:12:PHE:CD2	1:B:140:LEU:HD12	2.31	0.66
1:D:49:GLN:NE2	1:D:115:HIS:O	2.27	0.65
1:A:32:ASP:OD2	1:A:35:SER:OG	2.11	0.65
1:A:118:ILE:HG23	1:A:135:ARG:HE	1.60	0.65
1:C:122:THR:OG1	1:C:132:THR:OG1	2.14	0.65
1:E:79:GLN:CD	1:E:80:TRP:H	2.00	0.65
1:F:135:ARG:O	1:F:138:LEU:HD22	1.98	0.64
1:F:111:LEU:HD22	1:F:131:PHE:CD2	2.33	0.63
1:D:137:LEU:O	1:D:140:LEU:HD23	1.99	0.62
1:D:35:SER:OG	1:D:94:ASN:ND2	2.30	0.61
1:B:17:TYR:CD1	1:B:38:LEU:HD11	2.35	0.61
1:C:73:PHE:HB3	1:C:98:ALA:HB2	1.84	0.60
1:F:81:ILE:CG2	1:F:89:ALA:HB1	2.31	0.60
1:E:81:ILE:CG2	1:E:89:ALA:HB1	2.32	0.59
1:F:33:TRP:O	1:F:90:ARG:NH2	2.35	0.59
1:A:64:HIS:N	1:A:106:ASP:OD1	2.29	0.59
1:C:24:GLU:O	1:C:28:ALA:N	2.35	0.59
1:F:137:LEU:HD22	1:F:140:LEU:CD2	2.33	0.58
1:D:14:ILE:HG12	1:D:39:VAL:HG22	1.86	0.58
1:D:103:GLU:N	1:D:106:ASP:OD2	2.30	0.57
1:A:17:TYR:HD1	1:A:17:TYR:O	1.87	0.57
1:A:122:THR:OG1	1:A:132:THR:OG1	2.21	0.57
1:F:37:VAL:HG13	1:F:132:THR:HG21	1.84	0.57
1:B:18:HIS:HB3	1:B:87:TYR:CE1	2.39	0.56
1:A:81:ILE:HG23	1:A:90:ARG:N	2.20	0.56
1:D:73:PHE:N	1:D:73:PHE:CD1	2.71	0.56
1:A:13:LYS:HE2	1:A:15:ILE:HG21	1.86	0.56
1:A:62:CYS:O	1:A:66:ASP:N	2.39	0.55
1:A:118:ILE:HG23	1:A:135:ARG:NE	2.20	0.55
1:C:34:GLN:O	1:C:92:GLN:HG3	2.06	0.55
1:C:81:ILE:HA	1:C:90:ARG:O	2.07	0.55
1:A:10:GLY:O	1:A:46:GLY:N	2.30	0.54
1:C:82:GLU:O	1:C:89:ALA:HA	2.07	0.54
1:C:34:GLN:O	1:C:92:GLN:CG	2.56	0.54
1:F:22:ILE:O	1:F:26:GLN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLY:HA2	1:A:134:ILE:HG23	1.89	0.54
1:B:12:PHE:HD1	1:B:41:PRO:HA	1.74	0.54
1:E:81:ILE:HG23	1:E:89:ALA:HB1	1.89	0.53
1:E:103:GLU:HG3	1:E:104:ALA:N	2.21	0.53
1:B:17:TYR:HA	1:B:38:LEU:HD13	1.90	0.53
1:F:34:GLN:O	1:F:90:ARG:NH2	2.42	0.53
1:F:110:LEU:CD2	1:F:120:LEU:HD22	2.39	0.52
1:A:17:TYR:HD2	1:A:33:TRP:HA	1.74	0.52
1:C:118:ILE:HD13	1:C:135:ARG:HH21	1.74	0.52
1:D:10:GLY:O	1:D:46:GLY:N	2.35	0.52
1:B:103:GLU:N	1:B:106:ASP:OD2	2.37	0.51
1:E:73:PHE:HB3	1:E:98:ALA:HB2	1.92	0.51
1:C:55:CYS:O	1:C:135:ARG:NH2	2.42	0.51
1:B:102:ALA:O	1:B:125:GLY:CA	2.59	0.50
1:C:135:ARG:O	1:C:138:LEU:HD22	2.11	0.50
1:A:118:ILE:HG21	1:A:135:ARG:HH21	1.76	0.50
1:D:22:ILE:HG13	1:D:23:GLU:N	2.26	0.50
1:E:135:ARG:O	1:E:138:LEU:HD22	2.12	0.49
1:D:7:VAL:HG12	1:D:9:VAL:HG23	1.94	0.49
1:F:52:ARG:HB3	1:F:138:LEU:HD23	1.92	0.49
1:C:18:HIS:HB3	1:C:87:TYR:CZ	2.48	0.49
1:F:81:ILE:HG23	1:F:89:ALA:HB1	1.95	0.49
1:E:32:ASP:OD2	1:E:35:SER:OG	2.09	0.48
1:B:17:TYR:CE2	1:B:33:TRP:HD1	2.31	0.48
1:B:17:TYR:N	1:B:36:ASP:OD1	2.45	0.48
1:D:62:CYS:O	1:D:66:ASP:N	2.46	0.48
1:A:135:ARG:O	1:A:138:LEU:HD12	2.13	0.48
1:C:92:GLN:HB3	1:C:95:VAL:HG21	1.95	0.48
1:A:33:TRP:O	1:A:90:ARG:NH2	2.42	0.48
1:F:4:PHE:CE1	1:F:63:ARG:NH2	2.82	0.48
1:E:92:GLN:OE1	1:E:122:THR:HG21	2.13	0.47
1:B:122:THR:HG23	1:B:123:ALA:N	2.28	0.47
1:F:96:LEU:HB2	1:F:131:PHE:HB2	1.97	0.47
1:F:121:LEU:HA	1:F:131:PHE:HD1	1.79	0.47
1:B:22:ILE:O	1:B:26:GLN:N	2.41	0.47
1:B:102:ALA:O	1:B:125:GLY:HA2	2.14	0.47
1:C:64:HIS:ND1	1:C:106:ASP:OD2	2.43	0.47
1:C:113:CYS:SG	1:C:118:ILE:HD11	2.54	0.46
1:D:106:ASP:O	1:D:121:LEU:HD22	2.16	0.46
1:F:96:LEU:HD11	1:F:133:ASP:CA	2.45	0.46
1:B:125:GLY:N	1:B:128:ILE:O	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ILE:CG2	1:B:89:ALA:HB1	2.46	0.46
1:D:107:CYS:HA	1:D:121:LEU:CD2	2.45	0.46
1:B:39:VAL:HG11	1:B:140:LEU:HD11	1.97	0.46
1:F:92:GLN:OE1	1:F:122:THR:HG21	2.16	0.46
1:C:35:SER:HB2	1:C:37:VAL:HG12	1.97	0.46
1:E:17:TYR:HB3	1:E:87:TYR:OH	2.16	0.45
1:E:113:CYS:HB2	1:E:114:PRO:CD	2.46	0.45
1:D:39:VAL:HG11	1:D:140:LEU:HD11	1.99	0.45
1:A:17:TYR:O	1:A:17:TYR:CD1	2.68	0.45
1:B:12:PHE:HD2	1:B:140:LEU:HD12	1.80	0.45
1:A:21:THR:O	1:A:25:ARG:HG3	2.17	0.45
1:B:122:THR:CG2	1:B:123:ALA:N	2.80	0.45
1:E:22:ILE:H	1:E:22:ILE:HD12	1.82	0.44
1:A:64:HIS:ND1	1:A:106:ASP:OD2	2.49	0.44
1:B:137:LEU:O	1:B:140:LEU:HD23	2.17	0.44
1:F:84:THR:OG1	1:F:87:TYR:N	2.49	0.44
1:A:11:SER:HA	1:A:44:ALA:O	2.17	0.44
1:D:107:CYS:HA	1:D:121:LEU:HD23	2.00	0.44
1:F:133:ASP:OD2	1:F:135:ARG:NH1	2.51	0.44
1:A:60:TYR:OH	1:A:101:PRO:HD2	2.17	0.44
1:B:25:ARG:HD2	1:D:26:GLN:O	2.17	0.44
1:C:118:ILE:HG23	1:C:135:ARG:NE	2.32	0.44
1:D:31:VAL:HG22	1:D:38:LEU:HD23	1.99	0.44
1:F:13:LYS:HD2	1:F:15:ILE:HG23	2.00	0.44
1:F:110:LEU:HD22	1:F:120:LEU:CD2	2.48	0.44
1:A:103:GLU:OE2	1:A:103:GLU:HA	2.17	0.43
1:D:60:TYR:OH	1:D:101:PRO:O	2.23	0.43
1:E:139:TRP:HZ3	1:A:33:TRP:CZ3	2.36	0.43
1:C:17:TYR:N	1:C:36:ASP:OD1	2.51	0.43
1:D:137:LEU:HB3	1:D:140:LEU:HD23	1.98	0.43
1:D:52:ARG:CB	1:D:138:LEU:HD13	2.49	0.43
1:A:118:ILE:CG2	1:A:135:ARG:HH21	2.32	0.43
1:E:113:CYS:HB2	1:E:114:PRO:HD2	2.00	0.42
1:C:15:ILE:HD11	1:C:20:ALA:HA	2.01	0.42
1:C:81:ILE:HG23	1:C:89:ALA:HB1	2.00	0.42
1:A:17:TYR:N	1:A:36:ASP:OD1	2.53	0.42
1:F:96:LEU:HD11	1:F:133:ASP:N	2.34	0.42
1:F:110:LEU:HD23	1:F:120:LEU:HD22	1.99	0.42
1:E:136:ASN:OD1	1:E:136:ASN:N	2.52	0.42
1:F:13:LYS:HD2	1:F:15:ILE:CG2	2.50	0.42
1:F:39:VAL:HG11	1:F:140:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLN:NE2	1:B:91:TYR:O	2.51	0.42
1:D:106:ASP:C	1:D:121:LEU:HD22	2.40	0.41
1:A:81:ILE:HG22	1:C:141:ASP:C	2.40	0.41
1:B:12:PHE:CD2	1:B:140:LEU:CD1	3.00	0.41
1:B:17:TYR:HA	1:B:38:LEU:CD1	2.49	0.41
1:D:110:LEU:HD12	1:D:120:LEU:HD23	2.02	0.41
1:F:110:LEU:CD2	1:F:120:LEU:CD2	2.98	0.41
1:B:102:ALA:O	1:B:125:GLY:HA3	2.20	0.41
1:B:135:ARG:O	1:B:138:LEU:CD1	2.68	0.41
1:C:25:ARG:CZ	1:F:26:GLN:O	2.69	0.41
1:C:29:ILE:N	1:C:39:VAL:O	2.52	0.41
1:F:63:ARG:N	1:F:106:ASP:OD1	2.53	0.41
1:A:133:ASP:OD1	1:A:135:ARG:HG3	2.21	0.40
1:B:49:GLN:NE2	1:B:115:HIS:O	2.55	0.40
1:E:110:LEU:HD23	1:E:120:LEU:HD23	2.03	0.40
1:C:92:GLN:HB3	1:C:95:VAL:CG2	2.51	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	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	B	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	C	139/147 (95%)	135 (97%)	4 (3%)	0	100	100
1	D	140/147 (95%)	133 (95%)	7 (5%)	0	100	100
1	E	140/147 (95%)	138 (99%)	2 (1%)	0	100	100
1	F	140/147 (95%)	136 (97%)	4 (3%)	0	100	100
All	All	839/882 (95%)	816 (97%)	23 (3%)	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	94/115 (82%)	92 (98%)	2 (2%)	53	75
1	B	100/115 (87%)	100 (100%)	0	100	100
1	C	86/115 (75%)	86 (100%)	0	100	100
1	D	95/115 (83%)	93 (98%)	2 (2%)	53	75
1	E	99/115 (86%)	99 (100%)	0	100	100
1	F	91/115 (79%)	90 (99%)	1 (1%)	73	88
All	All	565/690 (82%)	560 (99%)	5 (1%)	78	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	TYR
1	A	49	GLN
1	D	73	PHE
1	D	82	GLU
1	F	11	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	F	83	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 ⓘ

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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	142/147 (96%)	0.72	13 (9%)	9	7	50, 74, 94, 111	0
1	B	142/147 (96%)	0.57	7 (4%)	29	26	49, 68, 89, 99	0
1	C	141/147 (95%)	0.64	11 (7%)	13	10	57, 78, 95, 101	0
1	D	142/147 (96%)	0.58	10 (7%)	16	13	52, 75, 89, 105	0
1	E	142/147 (96%)	0.54	5 (3%)	44	39	43, 61, 81, 93	0
1	F	142/147 (96%)	0.71	12 (8%)	10	8	56, 84, 99, 105	0
All	All	851/882 (96%)	0.63	58 (6%)	17	14	43, 74, 95, 111	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	LEU	8.1
1	A	142	THR	7.3
1	E	140	LEU	7.0
1	A	141	ASP	5.8
1	D	4	PHE	5.6
1	D	5	GLY	5.2
1	C	104	ALA	4.3
1	C	141	ASP	4.0
1	C	140	LEU	3.9
1	F	3	GLY	3.9
1	F	73	PHE	3.8
1	A	2	PRO	3.6
1	B	1	GLY	3.4
1	D	6	GLY	3.3
1	D	140	LEU	3.3
1	F	4	PHE	3.3
1	C	1	GLY	3.1
1	C	17	TYR	3.1
1	D	33	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	139	TRP	3.1
1	F	70	PRO	3.0
1	D	111	LEU	3.0
1	C	4	PHE	3.0
1	A	5	GLY	3.0
1	A	104	ALA	2.7
1	F	117	VAL	2.7
1	B	140	LEU	2.7
1	C	7	VAL	2.6
1	F	25	ARG	2.6
1	A	4	PHE	2.6
1	D	141	ASP	2.5
1	F	99	ALA	2.5
1	F	140	LEU	2.5
1	D	80	TRP	2.4
1	E	15	ILE	2.4
1	B	89	ALA	2.4
1	C	109	GLY	2.3
1	F	112	VAL	2.3
1	C	88	PRO	2.3
1	A	134	ILE	2.2
1	A	15	ILE	2.2
1	E	141	ASP	2.2
1	F	71	VAL	2.2
1	A	33	TRP	2.2
1	B	38	LEU	2.2
1	B	126	GLY	2.1
1	B	39	VAL	2.1
1	B	14	ILE	2.1
1	A	102	ALA	2.1
1	F	81	ILE	2.1
1	E	33	TRP	2.1
1	A	109	GLY	2.1
1	C	87	TYR	2.1
1	E	8	PHE	2.1
1	F	97	LEU	2.0
1	D	7	VAL	2.0
1	A	138	LEU	2.0
1	C	97	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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
2	ZN	F	201	1/1	0.94	0.13	90,90,90,90	0
2	ZN	A	201	1/1	0.95	0.17	82,82,82,82	0
2	ZN	C	201	1/1	0.97	0.15	77,77,77,77	0
2	ZN	B	201	1/1	0.98	0.17	67,67,67,67	0
2	ZN	D	201	1/1	0.99	0.13	84,84,84,84	0
2	ZN	E	201	1/1	0.99	0.14	77,77,77,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.