Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 04:07 PM EDT

PDB ID	:	6MAF
Title	:	native BbvCI A2B2 tetramer at low resolution
Authors	:	Shen, B.W.; Stoddard, B.L.
Deposited on	:	2018-08-27
Resolution	:	3.79 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (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 3.79 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.
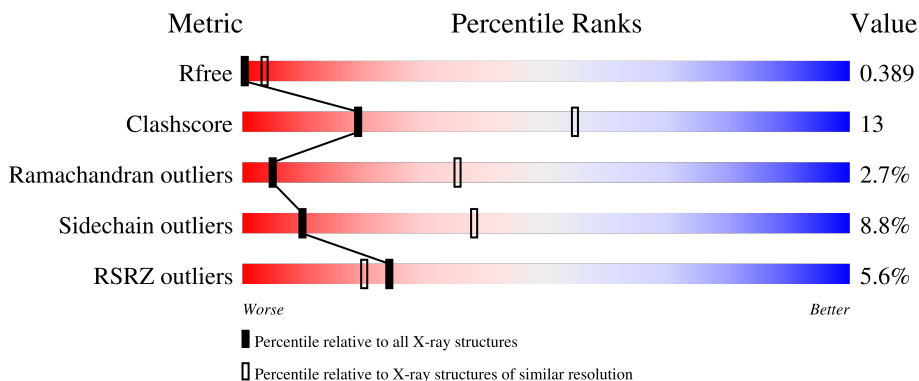
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	275	6% / 57% / 30% / 5% · 6%
1	B	275	6% / 57% / 30% / 5% · 6%
2	C	285	4% / 76% / 19% · ·
2	D	285	5% / 77% / 18% · ·

2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8630 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 BbvCI endonuclease subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2089	1329	361	395	4			
1	B	259	Total	C	N	O	S	0	0	0
			2089	1329	361	395	4			

- Molecule 2 is a protein called BbvCI endonuclease subunit 2.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	277	Total	C	N	O	S	0	0	0
			2226	1420	380	418	8			
2	D	277	Total	C	N	O	S	0	0	0
			2226	1420	380	418	8			

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.
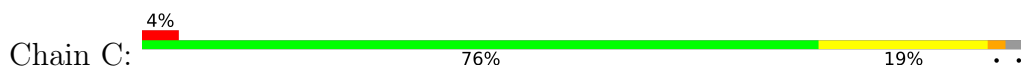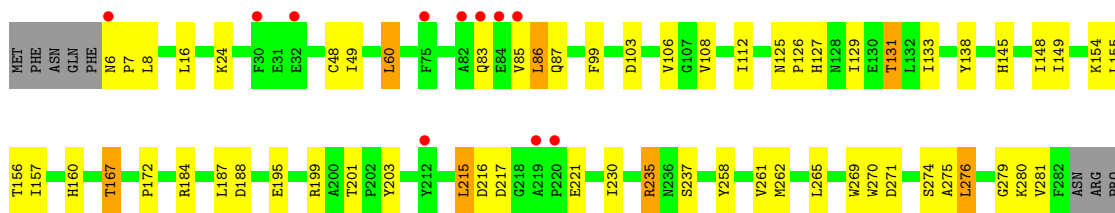
• Molecule 1: BbvCI endonuclease subunit 1
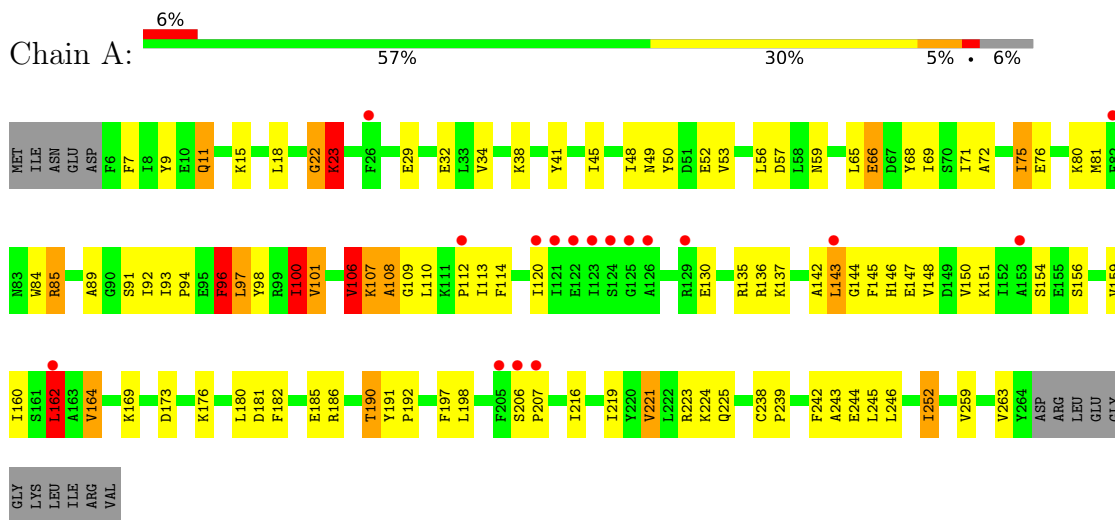
Chain A:
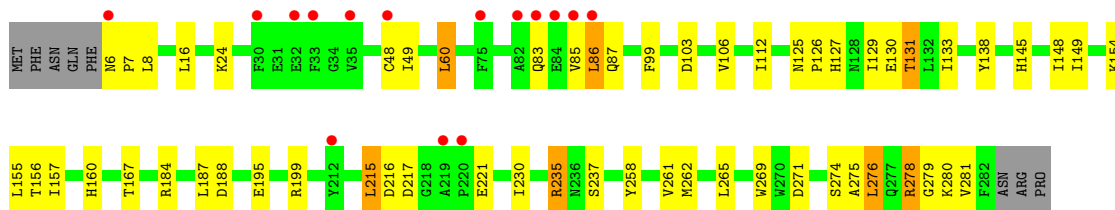

• Molecule 1: BbvCI endonuclease subunit 1
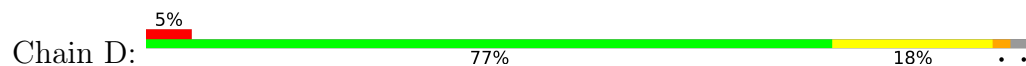
Chain B:

• Molecule 2: BbvCI endonuclease subunit 2

Chain C:
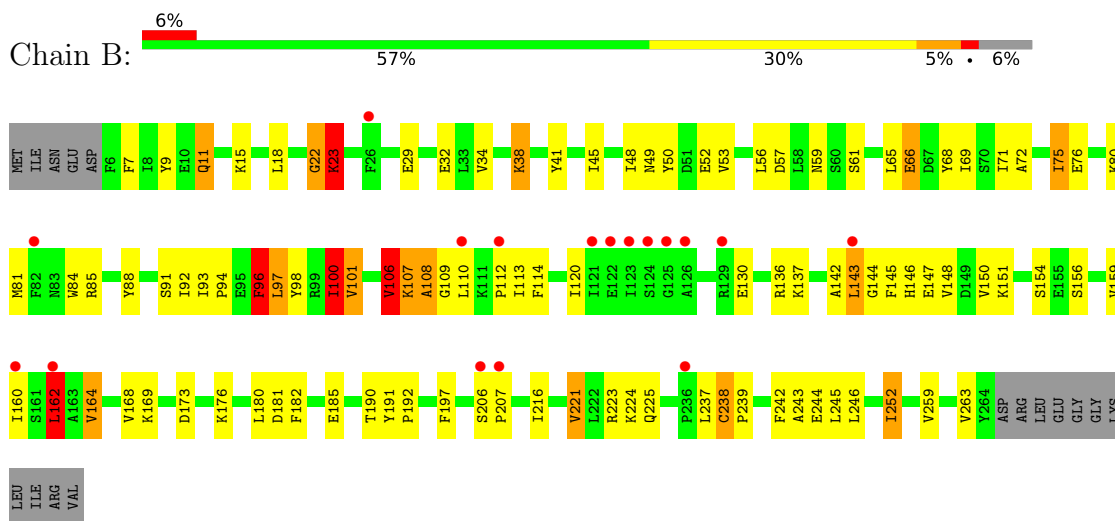
• Molecule 2: BbvCI endonuclease subunit 2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	113.15Å 113.15Å 115.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.40 – 3.79 28.40 – 3.79	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.40-3.79) 99.0 (28.40-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.297 , 0.388 0.300 , 0.389	Depositor DCC
R_{free} test set	768 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	113.5	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 109.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l 0.043 for h,-h-k,-l 0.438 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8630	wwPDB-VP
Average B, all atoms (Å^2)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 (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	0.53	0/2125	0.81	3/2856 (0.1%)
1	B	0.53	0/2125	0.82	5/2856 (0.2%)
2	C	0.56	0/2277	0.81	2/3082 (0.1%)
2	D	0.55	0/2277	0.81	2/3082 (0.1%)
All	All	0.54	0/8804	0.81	12/11876 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	18	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	162	LEU	CA-CB-CG	5.66	128.33	115.30
1	B	162	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	180	LEU	CA-CB-CG	5.54	128.05	115.30
2	C	86	LEU	CB-CA-C	-5.46	99.82	110.20
2	D	86	LEU	CB-CA-C	-5.46	99.83	110.20
1	A	180	LEU	CA-CB-CG	5.43	127.80	115.30
2	D	8	LEU	CA-CB-CG	5.20	127.25	115.30
2	C	8	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	18	LEU	CB-CG-CD1	5.08	119.64	111.00
1	B	237	LEU	CA-CB-CG	5.08	126.98	115.30

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	2089	0	2082	86	0
1	B	2089	0	2082	86	0
2	C	2226	0	2201	34	0
2	D	2226	0	2201	34	0
All	All	8630	0	8566	224	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 13.

All (224) 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:A:146:HIS:HB2	1:A:147:GLU:HB3	1.44	0.98
1:B:146:HIS:HB2	1:B:147:GLU:HB3	1.44	0.96
1:B:148:VAL:HG23	1:B:159:VAL:HB	1.46	0.96
1:A:148:VAL:HG23	1:A:159:VAL:HB	1.46	0.95
1:A:108:ALA:HB1	1:A:160:ILE:HD12	1.48	0.94
1:B:108:ALA:HB1	1:B:160:ILE:HD12	1.48	0.94
1:B:50:TYR:CD1	1:B:101:VAL:HG11	2.04	0.93
1:A:50:TYR:CD1	1:A:101:VAL:HG11	2.04	0.92
1:A:108:ALA:HB3	1:A:160:ILE:HG23	1.52	0.91
1:B:108:ALA:HB3	1:B:160:ILE:HG23	1.53	0.90
2:D:16:LEU:HD23	2:D:86:LEU:HD23	1.55	0.89
2:C:16:LEU:HD23	2:C:86:LEU:HD23	1.55	0.88
2:D:16:LEU:HD23	2:D:86:LEU:CD2	2.14	0.78
2:C:16:LEU:HD23	2:C:86:LEU:CD2	2.15	0.77
2:C:156:THR:HB	2:D:156:THR:HB	1.64	0.77
1:B:148:VAL:CG2	1:B:159:VAL:HB	2.16	0.74
1:A:148:VAL:CG2	1:A:159:VAL:HB	2.16	0.74
1:A:72:ALA:O	1:A:75:ILE:HG12	1.89	0.72
1:B:72:ALA:O	1:B:75:ILE:HG12	1.89	0.71
1:B:50:TYR:CG	1:B:101:VAL:HG11	2.25	0.70
1:A:50:TYR:CG	1:A:101:VAL:HG11	2.25	0.69
1:B:107:LYS:HG3	1:B:143:LEU:HD12	1.74	0.69
1:A:107:LYS:HG3	1:A:143:LEU:HD12	1.75	0.69
1:B:11:GLN:HB2	1:B:91:SER:O	1.93	0.68
1:B:50:TYR:CD1	1:B:101:VAL:CG1	2.76	0.68
1:A:100:ILE:HD13	1:A:100:ILE:H	1.58	0.68
1:A:50:TYR:CD1	1:A:101:VAL:CG1	2.76	0.68
1:B:52:GLU:HB3	1:B:57:ASP:CG	2.15	0.68
1:A:11:GLN:HB2	1:A:91:SER:O	1.92	0.68
1:B:72:ALA:HA	1:B:75:ILE:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HD13	1:B:100:ILE:H	1.58	0.68
1:A:151:LYS:HD2	1:B:151:LYS:HD2	1.76	0.67
1:A:52:GLU:HB3	1:A:57:ASP:CG	2.14	0.66
1:B:68:TYR:HE2	1:B:92:ILE:HD12	1.60	0.66
1:A:72:ALA:HA	1:A:75:ILE:HD11	1.76	0.66
1:A:68:TYR:HE2	1:A:92:ILE:HD12	1.61	0.66
1:B:107:LYS:HG2	1:B:143:LEU:HA	1.78	0.66
1:A:107:LYS:HG2	1:A:143:LEU:HA	1.79	0.65
2:C:269:TRP:HB2	2:D:126:PRO:O	1.97	0.65
1:A:151:LYS:HB3	1:B:151:LYS:HB3	1.77	0.64
2:C:258:TYR:O	2:C:262:MET:HG2	1.98	0.64
1:B:169:LYS:HE3	1:B:176:LYS:HE2	1.80	0.64
2:D:271:ASP:HB3	2:D:274:SER:HB3	1.79	0.63
2:D:258:TYR:O	2:D:262:MET:HG2	1.98	0.63
2:C:16:LEU:CD2	2:C:86:LEU:HD23	2.29	0.62
1:B:66:GLU:HA	1:B:69:ILE:HG22	1.82	0.62
2:C:271:ASP:HB3	2:C:274:SER:HB3	1.80	0.62
2:D:16:LEU:CD2	2:D:86:LEU:HD23	2.28	0.62
1:A:169:LYS:HE3	1:A:176:LYS:HE2	1.81	0.62
1:A:66:GLU:HA	1:A:69:ILE:HG22	1.82	0.62
1:B:120:ILE:HD13	1:B:130:GLU:HA	1.83	0.61
1:A:120:ILE:HD13	1:A:130:GLU:HA	1.83	0.60
1:B:223:ARG:HD3	1:B:239:PRO:HB3	1.84	0.60
1:A:151:LYS:HE2	1:A:154:SER:HA	1.84	0.60
1:A:223:ARG:HD3	1:A:239:PRO:HB3	1.84	0.60
1:B:151:LYS:HE2	1:B:154:SER:HA	1.84	0.60
2:C:126:PRO:O	2:D:269:TRP:HB2	2.01	0.60
1:A:223:ARG:HD3	1:A:239:PRO:CB	2.32	0.59
1:B:29:GLU:HG3	1:B:34:VAL:HB	1.85	0.59
1:B:173:ASP:OD1	1:B:176:LYS:HB3	2.03	0.59
1:A:29:GLU:HG3	1:A:34:VAL:HB	1.84	0.59
1:A:108:ALA:CB	1:A:160:ILE:HG23	2.29	0.59
1:B:15:LYS:NZ	1:B:38:LYS:HB2	2.17	0.59
1:B:223:ARG:HD3	1:B:239:PRO:CB	2.32	0.59
1:A:173:ASP:OD1	1:A:176:LYS:HB3	2.03	0.59
2:D:275:ALA:O	2:D:279:GLY:N	2.32	0.59
1:A:15:LYS:NZ	1:A:38:LYS:HB2	2.17	0.58
1:B:93:ILE:N	1:B:94:PRO:CD	2.66	0.58
1:A:93:ILE:N	1:A:94:PRO:CD	2.66	0.58
2:C:275:ALA:O	2:C:279:GLY:N	2.31	0.58
1:A:68:TYR:O	1:A:71:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TYR:O	1:B:71:ILE:HG12	2.04	0.57
1:B:108:ALA:CB	1:B:160:ILE:HG23	2.28	0.57
2:C:235:ARG:HD2	2:C:237:SER:H	1.69	0.57
1:B:182:PHE:O	1:B:185:GLU:HG2	2.04	0.57
1:B:114:PHE:CE1	1:B:137:LYS:HB2	2.40	0.57
2:D:235:ARG:HD2	2:D:237:SER:H	1.69	0.57
1:A:114:PHE:CE1	1:A:137:LYS:HB2	2.40	0.57
1:A:41:TYR:CE1	1:A:45:ILE:HD11	2.40	0.57
1:A:182:PHE:O	1:A:185:GLU:HG2	2.05	0.56
1:B:41:TYR:CE1	1:B:45:ILE:HD11	2.40	0.56
1:A:182:PHE:CE2	2:D:188:ASP:HB3	2.41	0.56
1:A:181:ASP:HA	1:A:216:ILE:HD11	1.88	0.56
1:B:146:HIS:CB	1:B:147:GLU:HB3	2.29	0.56
1:B:181:ASP:HA	1:B:216:ILE:HD11	1.87	0.55
2:D:274:SER:O	2:D:278:ARG:HB2	2.07	0.55
2:C:145:HIS:HD2	2:C:148:ILE:HD11	1.72	0.55
1:B:15:LYS:NZ	1:B:38:LYS:CB	2.70	0.54
2:C:138:TYR:CD1	2:C:157:ILE:HG13	2.42	0.54
1:B:182:PHE:CE2	2:C:188:ASP:HB3	2.43	0.54
1:A:15:LYS:NZ	1:A:38:LYS:CB	2.70	0.54
1:A:22:GLY:O	1:A:23:LYS:HB3	2.08	0.54
2:D:138:TYR:CD1	2:D:157:ILE:HG13	2.43	0.54
1:A:144:GLY:HA2	1:A:162:LEU:HA	1.90	0.53
1:B:242:PHE:HB3	1:B:245:LEU:HD23	1.90	0.53
2:C:133:ILE:O	2:C:160:HIS:HB2	2.07	0.53
1:A:15:LYS:HZ1	1:A:38:LYS:HB2	1.73	0.53
1:B:22:GLY:O	1:B:23:LYS:HB3	2.08	0.53
1:A:242:PHE:HB3	1:A:245:LEU:HD23	1.90	0.53
1:B:15:LYS:HZ1	1:B:38:LYS:HB2	1.72	0.53
1:B:56:LEU:HA	1:B:59:ASN:ND2	2.24	0.53
1:B:144:GLY:HA2	1:B:162:LEU:HA	1.90	0.53
2:D:145:HIS:HD2	2:D:148:ILE:HD11	1.72	0.53
1:A:56:LEU:HA	1:A:59:ASN:ND2	2.24	0.53
1:B:145:PHE:CE1	1:B:259:VAL:HB	2.45	0.52
2:D:133:ILE:O	2:D:160:HIS:HB2	2.08	0.52
1:A:114:PHE:O	1:A:190:THR:OG1	2.16	0.52
1:A:145:PHE:CE1	1:A:259:VAL:HB	2.45	0.52
2:D:85:VAL:C	2:D:86:LEU:HD12	2.31	0.51
2:C:85:VAL:C	2:C:86:LEU:HD12	2.31	0.51
1:B:150:VAL:O	1:B:156:SER:HA	2.11	0.51
1:A:150:VAL:O	1:A:156:SER:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:TYR:HH	2:C:270:TRP:HE3	1.59	0.50
1:A:106:VAL:O	1:A:107:LYS:HB2	2.12	0.50
1:B:59:ASN:HA	1:B:243:ALA:HB1	1.94	0.50
2:C:49:ILE:HD12	2:C:60:LEU:HD13	1.94	0.50
1:A:113:ILE:HD13	1:A:136:ARG:HB3	1.93	0.49
1:B:96:PHE:CD2	1:B:97:LEU:HD23	2.47	0.49
1:A:146:HIS:CB	1:A:147:GLU:HB3	2.29	0.49
1:B:113:ILE:HD13	1:B:136:ARG:HB3	1.93	0.49
2:D:85:VAL:O	2:D:86:LEU:HD12	2.13	0.49
1:A:32:GLU:OE2	1:A:80:LYS:HD2	2.11	0.49
1:B:148:VAL:O	1:B:159:VAL:O	2.31	0.49
2:D:49:ILE:HD12	2:D:60:LEU:HD13	1.94	0.49
2:C:85:VAL:O	2:C:86:LEU:HD12	2.13	0.49
1:A:96:PHE:CD2	1:A:97:LEU:HD23	2.48	0.49
1:B:41:TYR:CE1	1:B:65:LEU:HA	2.48	0.49
1:B:49:ASN:O	1:B:53:VAL:HG23	2.13	0.49
1:A:197:PHE:HE2	1:A:252:ILE:HB	1.78	0.49
1:B:32:GLU:OE2	1:B:80:LYS:HD2	2.12	0.49
1:A:59:ASN:HA	1:A:243:ALA:HB1	1.94	0.48
1:B:106:VAL:O	1:B:107:LYS:HB2	2.14	0.48
1:A:49:ASN:O	1:A:53:VAL:HG23	2.13	0.48
2:C:265:LEU:HD22	2:D:129:ILE:HD13	1.95	0.48
1:A:41:TYR:CE1	1:A:65:LEU:HA	2.48	0.48
1:B:225:GLN:HG3	1:B:239:PRO:HB3	1.95	0.48
1:A:56:LEU:HA	1:A:59:ASN:HD21	1.78	0.48
1:B:56:LEU:HA	1:B:59:ASN:HD21	1.78	0.48
1:A:221:VAL:O	1:A:245:LEU:HG	2.13	0.48
1:B:197:PHE:HE2	1:B:252:ILE:HB	1.79	0.48
1:B:221:VAL:O	1:B:245:LEU:HG	2.13	0.48
2:D:99:PHE:CE1	2:D:261:VAL:HG11	2.49	0.48
1:A:148:VAL:O	1:A:159:VAL:O	2.31	0.47
1:A:225:GLN:HG3	1:A:239:PRO:HB3	1.95	0.47
2:C:184:ARG:HH11	2:C:184:ARG:CB	2.27	0.47
2:D:184:ARG:CB	2:D:184:ARG:HH11	2.28	0.47
2:C:112:ILE:O	2:C:149:ILE:HA	2.14	0.47
2:D:112:ILE:O	2:D:149:ILE:HA	2.14	0.47
1:B:76:GLU:HG3	1:B:84:TRP:HB3	1.97	0.47
1:A:41:TYR:CZ	1:A:45:ILE:HD11	2.50	0.47
2:C:99:PHE:CE1	2:C:261:VAL:HG11	2.50	0.46
1:B:41:TYR:CZ	1:B:45:ILE:HD11	2.50	0.46
1:B:242:PHE:CE2	1:B:244:GLU:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:LEU:HD13	2:D:216:ASP:H	1.81	0.46
1:B:223:ARG:C	1:B:225:GLN:H	2.19	0.46
1:A:223:ARG:C	1:A:225:GLN:H	2.19	0.46
1:A:242:PHE:CE2	1:A:244:GLU:HB2	2.51	0.46
1:A:34:VAL:HG22	1:A:75:ILE:HD12	1.98	0.45
1:B:100:ILE:HD13	1:B:100:ILE:N	2.30	0.45
2:C:215:LEU:HD13	2:C:216:ASP:H	1.81	0.45
1:A:164:VAL:HG11	1:A:252:ILE:HG13	1.98	0.45
2:C:129:ILE:HD13	2:D:265:LEU:HD22	1.98	0.45
1:B:34:VAL:HG22	1:B:75:ILE:HD12	1.97	0.45
1:B:143:LEU:HB3	1:B:164:VAL:HG12	1.99	0.45
1:B:206:SER:HB3	1:B:207:PRO:HD3	1.99	0.45
1:A:206:SER:HB3	1:A:207:PRO:HD3	1.99	0.45
1:B:15:LYS:NZ	1:B:38:LYS:HG3	2.32	0.44
1:B:191:TYR:HA	1:B:192:PRO:HD2	1.81	0.44
1:B:242:PHE:HE2	1:B:244:GLU:HB2	1.82	0.44
1:A:143:LEU:HB3	1:A:164:VAL:HG12	1.99	0.44
1:A:15:LYS:NZ	1:A:38:LYS:HG3	2.32	0.44
1:A:76:GLU:HG3	1:A:84:TRP:HB3	2.00	0.44
2:C:184:ARG:HH11	2:C:184:ARG:HB3	1.82	0.44
1:B:146:HIS:C	1:B:147:GLU:HB3	2.38	0.44
1:A:146:HIS:C	1:A:147:GLU:HB3	2.38	0.44
2:C:155:LEU:HA	2:D:156:THR:O	2.17	0.44
1:B:107:LYS:CG	1:B:143:LEU:HD12	2.47	0.44
1:B:164:VAL:HG11	1:B:252:ILE:HG13	1.98	0.43
1:A:93:ILE:H	1:A:94:PRO:CD	2.32	0.43
1:A:242:PHE:HE2	1:A:244:GLU:HB2	1.82	0.43
1:A:100:ILE:HD13	1:A:100:ILE:N	2.30	0.43
2:D:6:ASN:ND2	2:D:103:ASP:HB2	2.34	0.43
1:B:93:ILE:H	1:B:94:PRO:HD3	1.83	0.43
2:D:145:HIS:CD2	2:D:148:ILE:HD11	2.53	0.43
2:D:184:ARG:HH11	2:D:184:ARG:HB3	1.81	0.43
2:C:108:VAL:HG11	2:D:130:GLU:HA	2.01	0.43
2:C:127:HIS:H	2:C:131:THR:HG21	1.84	0.43
1:A:182:PHE:CZ	2:D:188:ASP:HB3	2.54	0.42
1:B:75:ILE:HD11	1:B:88:TYR:OH	2.19	0.42
1:A:191:TYR:HA	1:A:192:PRO:HD2	1.79	0.42
2:D:127:HIS:H	2:D:131:THR:HG21	1.84	0.42
1:B:224:LYS:HG3	2:D:276:LEU:O	2.19	0.42
2:C:6:ASN:ND2	2:C:103:ASP:HB2	2.35	0.42
1:A:107:LYS:CG	1:A:143:LEU:HD12	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:HB3	1:B:108:ALA:H	1.62	0.42
1:A:96:PHE:HD2	1:A:97:LEU:HD23	1.84	0.42
1:B:109:GLY:O	1:B:142:ALA:HB3	2.20	0.42
2:C:138:TYR:HH	2:C:167:THR:HG1	1.65	0.42
1:A:93:ILE:H	1:A:94:PRO:HD3	1.84	0.41
1:A:198:LEU:HD23	1:A:219:ILE:HG12	2.03	0.41
1:A:48:ILE:HG23	1:A:57:ASP:HB3	2.02	0.41
1:A:109:GLY:O	1:A:142:ALA:HB3	2.20	0.41
1:B:41:TYR:HB2	1:B:68:TYR:HB2	2.01	0.41
1:A:107:LYS:HB3	1:A:108:ALA:H	1.63	0.41
1:A:107:LYS:HG2	1:A:144:GLY:H	1.86	0.41
1:B:96:PHE:HD2	1:B:97:LEU:HD23	1.84	0.41
1:A:41:TYR:HB2	1:A:68:TYR:HB2	2.01	0.41
1:B:93:ILE:H	1:B:94:PRO:CD	2.33	0.41
1:A:224:LYS:HG3	2:C:276:LEU:O	2.20	0.41
1:B:68:TYR:CE2	1:B:92:ILE:HD12	2.48	0.41
2:C:156:THR:O	2:D:155:LEU:HA	2.21	0.41
1:A:52:GLU:HB3	1:A:57:ASP:OD1	2.20	0.41
1:A:89:ALA:C	1:A:91:SER:H	2.24	0.41
1:B:48:ILE:HD13	1:B:61:SER:HB3	2.02	0.41
1:B:93:ILE:N	1:B:94:PRO:HD3	2.36	0.41
1:A:72:ALA:HA	1:A:75:ILE:CD1	2.47	0.41
1:A:135:ARG:HG3	1:A:186:ARG:HH22	1.86	0.41
1:B:107:LYS:HG2	1:B:144:GLY:H	1.86	0.41
1:B:238:CYS:HA	1:B:239:PRO:HD3	1.88	0.41
2:C:172:PRO:HD2	2:C:201:THR:HG21	2.03	0.40
1:B:48:ILE:HG23	1:B:57:ASP:HB3	2.02	0.40
1:B:182:PHE:CZ	2:C:188:ASP:HB3	2.55	0.40
2:D:184:ARG:HB3	2:D:184:ARG:NH1	2.36	0.40
1:B:93:ILE:HB	1:B:168:VAL:HG11	2.03	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	249/275 (90%)	201 (81%)	38 (15%)	10 (4%)	3	28
1	B	249/275 (90%)	202 (81%)	37 (15%)	10 (4%)	3	28
2	C	275/285 (96%)	253 (92%)	18 (6%)	4 (2%)	10	46
2	D	275/285 (96%)	254 (92%)	17 (6%)	4 (2%)	10	46
All	All	1048/1120 (94%)	910 (87%)	110 (10%)	28 (3%)	5	35

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	96	PHE
1	A	106	VAL
1	A	107	LYS
1	A	108	ALA
1	A	112	PRO
1	B	23	LYS
1	B	96	PHE
1	B	106	VAL
1	B	107	LYS
1	B	108	ALA
1	B	112	PRO
1	A	85	ARG
1	A	101	VAL
1	B	85	ARG
1	B	101	VAL
2	C	217	ASP
2	D	217	ASP
1	A	22	GLY
1	A	100	ILE
1	B	22	GLY
1	B	100	ILE
2	D	276	LEU
2	C	276	LEU
2	C	7	PRO
2	C	281	VAL
2	D	7	PRO
2	D	281	VAL

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	227/241 (94%)	204 (90%)	23 (10%)	7	32
1	B	227/241 (94%)	204 (90%)	23 (10%)	7	32
2	C	242/250 (97%)	224 (93%)	18 (7%)	13	44
2	D	242/250 (97%)	223 (92%)	19 (8%)	12	42
All	All	938/982 (96%)	855 (91%)	83 (9%)	10	38

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	9	TYR
1	A	11	GLN
1	A	23	LYS
1	A	66	GLU
1	A	75	ILE
1	A	81	MET
1	A	85	ARG
1	A	96	PHE
1	A	97	LEU
1	A	98	TYR
1	A	100	ILE
1	A	106	VAL
1	A	110	LEU
1	A	143	LEU
1	A	162	LEU
1	A	164	VAL
1	A	190	THR
1	A	221	VAL
1	A	238	CYS
1	A	246	LEU
1	A	252	ILE
1	A	263	VAL
1	B	7	PHE

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Mol	Chain	Res	Type
1	B	9	TYR
1	B	11	GLN
1	B	23	LYS
1	B	38	LYS
1	B	66	GLU
1	B	75	ILE
1	B	81	MET
1	B	96	PHE
1	B	97	LEU
1	B	98	TYR
1	B	100	ILE
1	B	106	VAL
1	B	110	LEU
1	B	143	LEU
1	B	162	LEU
1	B	164	VAL
1	B	190	THR
1	B	221	VAL
1	B	238	CYS
1	B	246	LEU
1	B	252	ILE
1	B	263	VAL
2	C	24	LYS
2	C	48	CYS
2	C	60	LEU
2	C	83	GLN
2	C	87	GLN
2	C	106	VAL
2	C	125	ASN
2	C	131	THR
2	C	154	LYS
2	C	167	THR
2	C	187	LEU
2	C	195	GLU
2	C	199	ARG
2	C	215	LEU
2	C	221	GLU
2	C	230	ILE
2	C	235	ARG
2	C	280	LYS
2	D	24	LYS
2	D	48	CYS

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Mol	Chain	Res	Type
2	D	60	LEU
2	D	83	GLN
2	D	87	GLN
2	D	106	VAL
2	D	125	ASN
2	D	131	THR
2	D	154	LYS
2	D	167	THR
2	D	187	LEU
2	D	195	GLU
2	D	199	ARG
2	D	215	LEU
2	D	221	GLU
2	D	230	ILE
2	D	235	ARG
2	D	278	ARG
2	D	280	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	230	ASN
1	A	233	GLN
1	B	225	GLN
1	B	230	ASN
1	B	233	GLN
2	C	6	ASN
2	C	50	GLN
2	C	87	GLN
2	C	125	ASN
2	C	127	HIS
2	C	160	HIS
2	C	185	ASN
2	D	6	ASN
2	D	50	GLN
2	D	87	GLN
2	D	125	ASN
2	D	127	HIS
2	D	160	HIS
2	D	185	ASN

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
1	B	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	146:HIS	C	147:GLU	N	4.93
1	B	146:HIS	C	147:GLU	N	4.93
1	A	53:VAL	C	54:THR	N	3.17
1	B	53:VAL	C	54:THR	N	3.17
1	A	148:VAL	C	149:ASP	N	3.15
1	B	148:VAL	C	149:ASP	N	3.15
1	A	158:ARG	C	159:VAL	N	3.10
1	B	158:ARG	C	159:VAL	N	3.09

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	259/275 (94%)	0.34	17 (6%)	18	14	67, 182, 373, 500	0
1	B	259/275 (94%)	0.31	17 (6%)	18	14	66, 182, 365, 500	0
2	C	277/285 (97%)	0.04	11 (3%)	38	32	51, 145, 279, 466	0
2	D	277/285 (97%)	0.09	15 (5%)	25	22	52, 149, 279, 482	0
All	All	1072/1120 (95%)	0.19	60 (5%)	24	20	51, 167, 331, 500	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	SER	13.7
1	B	206	SER	11.7
1	A	207	PRO	9.8
1	B	124	SER	7.2
2	D	84	GLU	7.1
1	A	122	GLU	7.0
1	A	121	ILE	6.8
1	A	124	SER	6.6
1	A	123	ILE	6.4
2	C	6	ASN	6.1
2	C	84	GLU	5.8
2	D	83	GLN	5.8
1	B	207	PRO	5.8
1	B	112	PRO	5.6
1	B	122	GLU	5.3
2	C	83	GLN	5.1
2	D	6	ASN	4.5
1	B	121	ILE	4.5
1	B	236	PRO	4.4
1	A	112	PRO	4.4
1	B	129	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	123	ILE	4.2
1	B	26	PHE	4.0
2	D	82	ALA	3.9
1	A	125	GLY	3.9
1	A	129	ARG	3.7
2	C	82	ALA	3.4
1	A	126	ALA	3.3
2	C	212	TYR	3.3
1	A	162	LEU	3.2
2	C	75	PHE	3.2
1	B	125	GLY	3.1
1	A	26	PHE	3.1
2	D	212	TYR	3.1
2	C	219	ALA	2.9
1	A	153	ALA	2.8
2	C	30	PHE	2.8
2	D	30	PHE	2.8
2	D	219	ALA	2.8
1	B	110	LEU	2.7
2	D	85	VAL	2.7
2	D	32	GLU	2.6
2	D	75	PHE	2.6
1	B	160	ILE	2.6
2	C	32	GLU	2.5
1	B	162	LEU	2.4
1	A	82	PHE	2.3
1	B	126	ALA	2.3
1	A	143	LEU	2.2
1	A	120	ILE	2.1
2	C	220	PRO	2.1
2	D	86	LEU	2.1
1	B	82	PHE	2.1
2	D	220	PRO	2.1
1	A	205	PHE	2.1
2	D	35	VAL	2.1
1	B	143	LEU	2.1
2	C	85	VAL	2.1
2	D	48	CYS	2.1
2	D	33	PHE	2.1

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 ⓘ

There are no ligands in this entry.

6.5　Other polymers ⓘ

There are no such residues in this entry.