



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:52 PM UTC

PDB ID : 2ZF3 / pdb_00002zf3
Title : Crystal Structure of VioE
Authors : Hirano, S.; Shiro, Y.; Nagano, S.
Deposited on : 2007-12-20
Resolution : 2.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

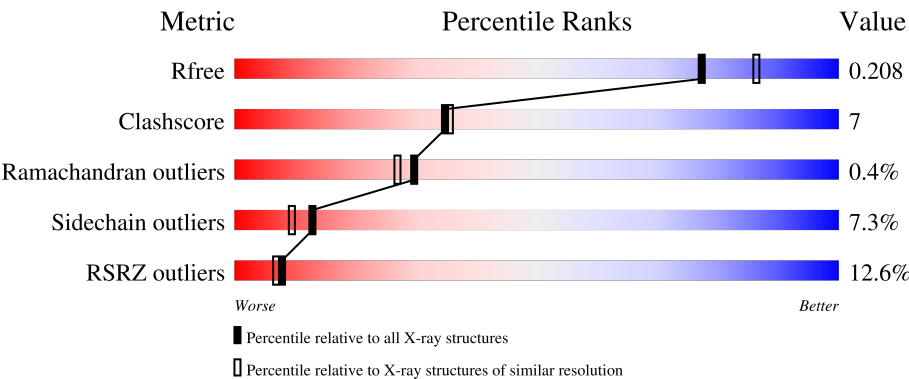
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	194	5% 88% 7% . .
1	B	194	12% 66% 18% . 13%
1	C	194	26% 69% 20% . 6%
1	D	194	7% 78% 15% . 5%
1	E	194	5% 81% 12% . .

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Mol	Chain	Length	Quality of chain
1	F	194	15% 74% 16% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9305 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 Hypothetical protein VioE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	3	0
			1518	955	278	279	6			
1	B	169	Total	C	N	O	S	0	6	0
			1384	878	246	253	7			
1	C	182	Total	C	N	O	S	0	2	0
			1474	929	268	269	8			
1	D	185	Total	C	N	O	S	0	5	0
			1502	949	267	279	7			
1	E	186	Total	C	N	O	S	0	1	0
			1495	941	271	276	7			
1	F	181	Total	C	N	O	S	0	1	0
			1455	914	263	271	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q7NSZ5
A	-1	SER	-	expression tag	UNP Q7NSZ5
A	0	HIS	-	expression tag	UNP Q7NSZ5
B	-2	GLY	-	expression tag	UNP Q7NSZ5
B	-1	SER	-	expression tag	UNP Q7NSZ5
B	0	HIS	-	expression tag	UNP Q7NSZ5
C	-2	GLY	-	expression tag	UNP Q7NSZ5
C	-1	SER	-	expression tag	UNP Q7NSZ5
C	0	HIS	-	expression tag	UNP Q7NSZ5
D	-2	GLY	-	expression tag	UNP Q7NSZ5
D	-1	SER	-	expression tag	UNP Q7NSZ5
D	0	HIS	-	expression tag	UNP Q7NSZ5
E	-2	GLY	-	expression tag	UNP Q7NSZ5
E	-1	SER	-	expression tag	UNP Q7NSZ5
E	0	HIS	-	expression tag	UNP Q7NSZ5
F	-2	GLY	-	expression tag	UNP Q7NSZ5
F	-1	SER	-	expression tag	UNP Q7NSZ5

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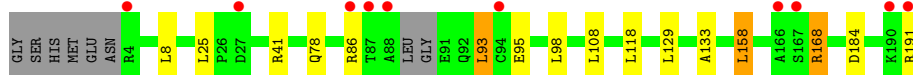
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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP Q7NSZ5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total	O	0	0
			150	150		
2	B	75	Total	O	0	0
			75	75		
2	C	70	Total	O	0	0
			70	70		
2	D	47	Total	O	0	0
			47	47		
2	E	65	Total	O	0	0
			65	65		
2	F	70	Total	O	0	0
			70	70		

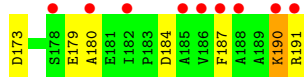
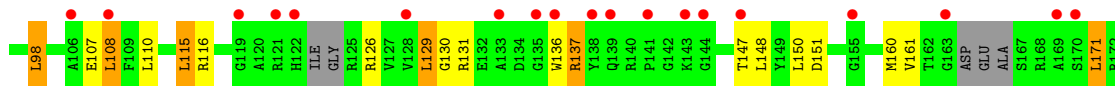
- Molecule 1: Hypothetical protein VioE



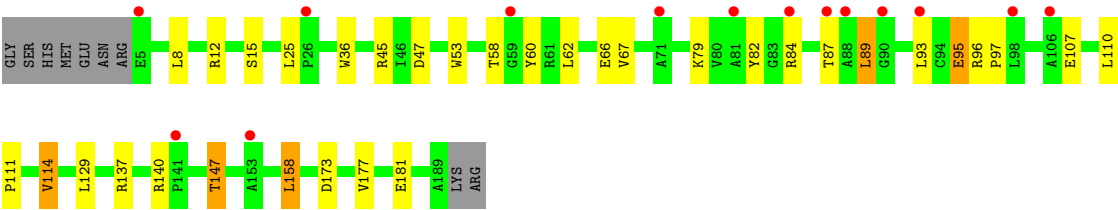
Label	Value	Color
GLY	1.00	Grey
HIS	1.00	Grey
HIS	1.00	Grey
MET	1.00	Grey
GLU	1.00	Grey
ASN	1.00	Grey
ARG	1.00	Grey
E5	1.00	Yellow
P6	1.00	Green
M24	1.00	Yellow
L25	1.00	Yellow
F26	1.00	Red
D27	1.00	Red
D28	1.00	Yellow
Y39	1.00	Yellow
F40	1.00	Yellow
R41	1.00	Yellow
D42	1.00	Yellow
R45	1.00	Yellow
P52	1.00	Red
TRP	1.00	Grey
SER	1.00	Grey
GLU	1.00	Grey
ARG	1.00	Grey
ASP	1.00	Grey
T58	1.00	Green
M64	1.00	Yellow
S65	1.00	Yellow
E66	1.00	Yellow
A70	1.00	Red
A71	1.00	Red
G72	1.00	Red
S73	1.00	Red
R74	1.00	Red
T75	1.00	Red
W76	1.00	Red
K77	1.00	Red
Q78	1.00	Red
T87	1.00	Red
ALA	1.00	Grey
LEU	1.00	Grey
G90	1.00	Red
C94	1.00	Yellow
E95	1.00	Yellow
G103	1.00	Red
F104	1.00	Red
F105	1.00	Red
ALA	1.00	Grey
GLU	1.00	Grey
L108	1.00	Red
L109	1.00	Red



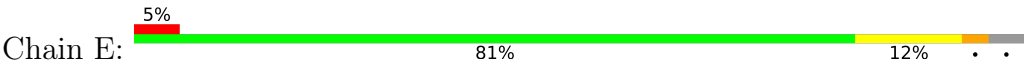
GLY	SER	HIS	MET	GLU	ASN	ARG	ASP	THR	VAL	PRO	LEU	PHE	TYP	CYS	TRP	LYS	ALA	GLN	ILE	TYR	DEU	HAU	GLY																	
E5	F6	P7	L8	I9	F10	A11	R12	W21	S22	P23	M24	L25	P26	D27	D28	Q29	L30	W36	E40	R41	D42	I43	C44	R45	T46	D47	F50	D57	S65	E66	V67	A70	A71	W76	V80	A81	E85	A88	G94	G95



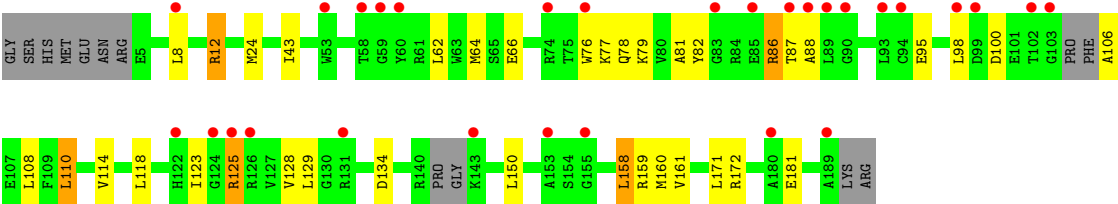
WORLD WIDE
PDB
PROTEIN DATA BANK



● Molecule 1: Hypothetical protein VioE



● Molecule 1: Hypothetical protein VioE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.10Å 88.44Å 153.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.25 – 2.00 39.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.25-2.00) 99.8 (39.25-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.245 0.210 , 0.208	Depositor DCC
R_{free} test set	3922 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9305	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.65	0/1568	0.79	0/2125
1	B	0.65	0/1436	0.81	2/1944 (0.1%)
1	C	0.60	1/1520 (0.1%)	0.86	2/2059 (0.1%)
1	D	0.56	0/1559	0.78	2/2119 (0.1%)
1	E	0.60	0/1540	0.78	0/2092
1	F	0.58	0/1495	0.76	0/2027
All	All	0.61	1/9118 (0.0%)	0.80	6/12366 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	57	ASP	CG-OD1	5.92	1.36	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	SER	CA-C-N	-9.33	110.10	119.90
1	C	22	SER	C-N-CA	-9.33	110.10	119.90
1	B	144	GLY	CA-C-N	5.85	127.16	119.84
1	B	144	GLY	C-N-CA	5.85	127.16	119.84
1	D	140	ARG	CA-C-N	5.10	124.81	119.82
1	D	140	ARG	C-N-CA	5.10	124.81	119.82

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	1518	0	1469	12	0
1	B	1384	0	1344	28	0
1	C	1474	0	1424	32	0
1	D	1502	0	1453	22	0
1	E	1495	0	1437	18	0
1	F	1455	0	1396	27	0
2	A	150	0	0	2	0
2	B	75	0	0	2	0
2	C	70	0	0	0	0
2	D	47	0	0	2	0
2	E	65	0	0	0	0
2	F	70	0	0	4	0
All	All	9305	0	8523	130	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 (130) 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:168:ARG:HG2	1:A:168:ARG:HH11	1.19	1.07
1:C:21:TRP:O	1:C:24:MET:HE2	1.65	0.96
1:C:95:GLU:HG3	1:D:129[A]:LEU:HD12	1.49	0.93
1:A:168:ARG:HH11	1:A:168:ARG:CG	1.87	0.88
1:E:56:ARG:HH11	1:E:56:ARG:HG3	1.39	0.87
1:E:17:TYR:CD1	1:E:172:ARG:HD2	2.09	0.86
1:B:147:THR:HG23	1:B:161:VAL:HB	1.63	0.81
1:D:111:PRO:HD2	1:D:114:VAL:CG1	2.11	0.80
1:D:58:THR:HG23	1:D:60:TYR:H	1.46	0.77
1:B:64:MET:HE3	1:B:66[B]:GLU:OE2	1.85	0.77
1:B:111:PRO:HD2	1:B:114:VAL:CG1	2.15	0.76
1:F:160[B]:MET:HE3	1:F:172:ARG:HG3	1.69	0.74
1:C:24:MET:HE1	1:D:93:LEU:HG	1.69	0.74
1:D:53:TRP:HE1	1:D:58:THR:HG21	1.54	0.73
1:F:62:LEU:HD21	1:F:64:MET:HE3	1.71	0.72
1:D:45:ARG:HD3	1:D:47:ASP:OD1	1.89	0.72
1:C:45:ARG:HG3	1:C:67:VAL:HG22	1.72	0.70
1:B:114:VAL:HG23	1:B:115:LEU:HD13	1.73	0.70
1:D:36:TRP:CZ3	1:D:45:ARG:HD2	2.27	0.69
1:D:137:ARG:HH21	1:D:147:THR:HG21	1.60	0.66
1:F:64:MET:HE2	1:F:79:LYS:HE2	1.77	0.66
1:C:45:ARG:HD3	1:C:47:ASP:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLN:NE2	1:A:191:ARG:HG3	2.11	0.65
1:F:66:GLU:HG3	2:F:225:HOH:O	1.95	0.65
1:E:81:ALA:HB3	1:E:96:ARG:HG3	1.77	0.65
1:D:87:THR:HG23	1:D:89:LEU:H	1.60	0.65
1:E:28:ASP:CG	1:E:168:ARG:HH22	2.06	0.64
1:D:53:TRP:NE1	1:D:58:THR:HG21	2.11	0.64
1:C:9:LEU:HD21	1:C:110:LEU:HG	1.79	0.64
1:E:126:ARG:NH2	1:E:159:ARG:HH11	1.96	0.63
1:C:148:LEU:HD13	1:C:160[A]:MET:HE2	1.80	0.63
1:F:64:MET:HE2	1:F:79:LYS:HG2	1.81	0.63
1:C:24:MET:HG2	1:C:28:ASP:CB	2.29	0.62
1:B:5:GLU:HG2	1:B:6:PRO:HD2	1.80	0.62
1:E:28:ASP:OD2	1:E:168:ARG:NH2	2.33	0.61
1:D:62:LEU:HD11	1:D:79:LYS:HB3	1.83	0.61
1:F:158:LEU:HD12	2:F:233:HOH:O	2.01	0.61
1:D:45:ARG:HG3	1:D:67:VAL:HG22	1.84	0.60
1:E:150:LEU:HD12	1:E:157:PRO:HA	1.84	0.59
1:F:12:ARG:HG2	2:F:212:HOH:O	2.00	0.59
1:B:146:SER:HB2	1:B:160[B]:MET:CE	2.33	0.59
1:C:41:ARG:NH2	1:C:184:ASP:OD1	2.35	0.58
1:D:66[B]:GLU:HG2	2:D:224:HOH:O	2.02	0.58
1:B:111:PRO:HD2	1:B:114:VAL:HG11	1.85	0.58
1:D:111:PRO:HD2	1:D:114:VAL:HG13	1.85	0.58
1:F:87:THR:HG22	1:F:88:ALA:H	1.68	0.57
1:E:126:ARG:HH22	1:E:159:ARG:HH11	1.53	0.57
1:C:161:VAL:HG22	1:C:171:LEU:HD13	1.85	0.56
1:C:6:PRO:HB2	1:C:115:LEU:HB3	1.88	0.56
1:F:82:TYR:CE1	1:F:95:GLU:HB3	2.41	0.56
1:C:24:MET:HG2	1:C:28:ASP:HB2	1.88	0.55
1:D:12:ARG:HD3	1:D:181:GLU:HA	1.88	0.55
1:A:168:ARG:CG	1:A:168:ARG:NH1	2.57	0.55
1:A:168:ARG:HG2	1:A:168:ARG:NH1	2.01	0.54
1:C:130:GLY:HA3	1:D:97:PRO:HG3	1.87	0.54
1:F:161:VAL:HG22	1:F:171:LEU:CD1	2.38	0.54
1:C:24:MET:HG2	1:C:28:ASP:HB3	1.89	0.54
1:E:107:GLU:HG3	1:E:111:PRO:HG3	1.89	0.53
1:C:36:TRP:CZ3	1:C:45:ARG:HD2	2.43	0.53
1:B:109:PHE:HA	2:B:261:HOH:O	2.07	0.53
1:C:12:ARG:HG3	1:C:12:ARG:HH11	1.73	0.53
1:D:129[B]:LEU:HD11	1:D:173:ASP:HB3	1.91	0.53
1:E:148:LEU:HG	1:E:150:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:LEU:HD13	1:F:24:MET:HG3	1.90	0.51
1:F:161:VAL:HG22	1:F:171:LEU:HD13	1.93	0.51
1:C:81:ALA:HB2	1:C:98:LEU:HD21	1.93	0.51
1:B:39:TYR:CD2	1:B:112:ARG:HG3	2.46	0.50
1:B:28:ASP:CG	1:B:168[B]:ARG:HH22	2.19	0.50
1:F:62:LEU:HD21	1:F:64:MET:CE	2.38	0.50
1:E:56:ARG:HH11	1:E:56:ARG:CG	2.18	0.50
1:F:77:LYS:O	1:F:100:ASP:HA	2.11	0.50
1:E:54:SER:HB3	1:E:57:ASP:OD2	2.12	0.50
1:E:56:ARG:HG3	1:E:56:ARG:NH1	2.15	0.49
1:C:129:LEU:N	1:D:95:GLU:OE2	2.42	0.49
1:F:81:ALA:O	1:F:95:GLU:HA	2.13	0.48
1:E:87:THR:HG22	1:E:88:ALA:H	1.79	0.48
1:A:93:LEU:HD13	1:B:24:MET:HG3	1.95	0.48
1:C:12:ARG:NH1	1:C:179:GLU:O	2.47	0.48
1:C:43:ILE:HD13	1:C:187:PHE:HB3	1.96	0.48
1:F:128:VAL:HG12	1:F:129:LEU:HD22	1.95	0.47
1:A:191:ARG:NH2	2:A:330:HOH:O	2.46	0.47
1:F:158:LEU:CD1	2:F:233:HOH:O	2.62	0.47
1:F:125:ARG:NH1	1:F:134:ASP:OD1	2.48	0.47
1:B:41:ARG:NH1	1:B:184[A]:ASP:OD2	2.48	0.47
1:B:111:PRO:HD2	1:B:114:VAL:HG13	1.95	0.47
1:C:137:ARG:HD3	1:C:147:THR:OG1	2.14	0.47
1:D:82:TYR:CE2	1:D:95:GLU:HB2	2.50	0.47
1:C:22:SER:OG	1:C:23:PRO:HD3	2.15	0.47
1:C:129:LEU:HD21	1:C:173:ASP:HB3	1.97	0.47
1:C:70:ALA:HB2	1:C:108:LEU:HD13	1.97	0.47
1:A:133:ALA:HB2	1:A:158:LEU:HD23	1.98	0.46
1:B:64:MET:HE3	1:B:66[B]:GLU:CD	2.40	0.46
1:B:76:TRP:CH2	1:B:78:GLN:HB2	2.49	0.46
1:B:158:LEU:HD13	2:B:194:HOH:O	2.15	0.46
1:C:136:TRP:CE3	1:C:150:LEU:HD23	2.51	0.46
1:D:158:LEU:HD13	2:D:221:HOH:O	2.15	0.46
1:B:108:LEU:HD22	1:B:108:LEU:N	2.31	0.46
1:F:76:TRP:CH2	1:F:78:GLN:HB2	2.50	0.46
1:F:86:ARG:HD2	1:F:86:ARG:HA	1.70	0.46
1:C:24:MET:CE	1:D:93:LEU:HG	2.41	0.45
1:C:6:PRO:HG2	1:C:116:ARG:HG2	1.99	0.45
1:A:129:LEU:HA	1:B:95:GLU:OE2	2.17	0.44
1:B:110:LEU:HD21	1:B:160[A]:MET:SD	2.58	0.44
1:C:9:LEU:CD2	1:C:110:LEU:HG	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:LYS:HD3	1:C:191:ARG:N	2.33	0.43
1:F:66:GLU:OE2	1:F:106:ALA:HA	2.18	0.43
1:B:146:SER:HB2	1:B:160[B]:MET:HE2	1.99	0.43
1:D:15:SER:HB2	1:D:177:VAL:HG22	2.00	0.43
1:B:123:ILE:HG22	1:B:124:GLY:H	1.84	0.43
1:C:131:ARG:HG2	1:C:151:ASP:OD1	2.18	0.43
1:F:159:ARG:HD3	1:F:171:LEU:HD12	2.01	0.43
1:F:114:VAL:O	1:F:118:LEU:HB2	2.19	0.42
1:A:95:GLU:CD	1:B:159:ARG:HH22	2.28	0.42
1:F:110:LEU:HD11	1:F:160[B]:MET:SD	2.60	0.41
1:E:54:SER:CB	1:E:57:ASP:OD2	2.69	0.41
1:F:64:MET:CE	1:F:79:LYS:HE2	2.45	0.41
1:A:41:ARG:NH2	1:A:184:ASP:OD1	2.53	0.41
1:F:181:GLU:O	1:F:181:GLU:HG3	2.20	0.41
1:C:43:ILE:HD11	1:C:67:VAL:CG1	2.50	0.41
1:B:150:LEU:HD12	1:B:157:PRO:HA	2.03	0.41
1:C:12:ARG:NH1	1:C:180:ALA:C	2.78	0.41
1:E:148:LEU:HD13	1:E:160[A]:MET:HE2	2.02	0.41
1:B:160[B]:MET:HE3	1:B:161:VAL:O	2.21	0.41
1:E:56:ARG:CG	1:E:56:ARG:NH1	2.80	0.41
1:F:87:THR:HG22	1:F:88:ALA:N	2.33	0.41
1:B:6:PRO:HB3	1:B:115:LEU:HB3	2.02	0.40
1:B:42:ASP:OD1	1:B:108:LEU:HD21	2.20	0.40
1:B:122:HIS:HB2	1:B:136:TRP:CZ3	2.56	0.40
1:A:191:ARG:HD3	2:A:240:HOH:O	2.21	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	185/194 (95%)	180 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	163/194 (84%)	157 (96%)	4 (2%)	2 (1%)	10	6
1	C	178/194 (92%)	170 (96%)	7 (4%)	1 (1%)	21	17
1	D	188/194 (97%)	178 (95%)	10 (5%)	0	100	100
1	E	185/194 (95%)	180 (97%)	5 (3%)	0	100	100
1	F	176/194 (91%)	173 (98%)	2 (1%)	1 (1%)	21	17
All	All	1075/1164 (92%)	1038 (97%)	33 (3%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	PRO
1	C	22	SER
1	B	124	GLY
1	F	123	ILE

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	157/160 (98%)	148 (94%)	9 (6%)	18	15
1	B	146/160 (91%)	137 (94%)	9 (6%)	16	13
1	C	153/160 (96%)	139 (91%)	14 (9%)	8	5
1	D	157/160 (98%)	146 (93%)	11 (7%)	14	10
1	E	154/160 (96%)	141 (92%)	13 (8%)	10	7
1	F	150/160 (94%)	140 (93%)	10 (7%)	15	11
All	All	917/960 (96%)	851 (93%)	66 (7%)	13	10

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	86	ARG
1	A	93	LEU
1	A	98	LEU
1	A	108	LEU
1	A	118	LEU
1	A	158	LEU
1	A	168	ARG
1	B	25	LEU
1	B	87	THR
1	B	108	LEU
1	B	115	LEU
1	B	117	ARG
1	B	147	THR
1	B	150	LEU
1	B	158	LEU
1	B	171	LEU
1	C	8	LEU
1	C	24	MET
1	C	30	LEU
1	C	40	GLU
1	C	85	GLU
1	C	98	LEU
1	C	107	GLU
1	C	108	LEU
1	C	115	LEU
1	C	126	ARG
1	C	129	LEU
1	C	137	ARG
1	C	171	LEU
1	C	190	LYS
1	D	8	LEU
1	D	25	LEU
1	D	84	ARG
1	D	89	LEU
1	D	95	GLU
1	D	96	ARG
1	D	107	GLU
1	D	110	LEU
1	D	114	VAL
1	D	147	THR
1	D	158	LEU
1	E	8	LEU

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Mol	Chain	Res	Type
1	E	25	LEU
1	E	40	GLU
1	E	49	LEU
1	E	56	ARG
1	E	89	LEU
1	E	91	GLU
1	E	93	LEU
1	E	98	LEU
1	E	131	ARG
1	E	150	LEU
1	E	168	ARG
1	E	172	ARG
1	F	8	LEU
1	F	12	ARG
1	F	43	ILE
1	F	86	ARG
1	F	98	LEU
1	F	108	LEU
1	F	110	LEU
1	F	125	ARG
1	F	150	LEU
1	F	158	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	B	92	GLN
1	D	92	GLN
1	E	139	GLN
1	F	92	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 [i](#)

There are no oligosaccharides 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, 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(Å ²)	Q < 0.9
1	A	186/194 (95%)	0.53	10 (5%)	31 30	14, 26, 39, 53	3 (1%)
1	B	169/194 (87%)	1.12	24 (14%)	6 5	13, 28, 41, 48	6 (3%)
1	C	182/194 (93%)	1.51	50 (27%)	1 1	15, 27, 37, 46	2 (1%)
1	D	185/194 (95%)	0.78	14 (7%)	20 18	12, 28, 39, 48	5 (2%)
1	E	186/194 (95%)	0.53	10 (5%)	31 30	16, 28, 38, 40	1 (0%)
1	F	181/194 (93%)	0.94	29 (16%)	5 4	16, 28, 43, 53	1 (0%)
All	All	1089/1164 (93%)	0.90	137 (12%)	8 7	12, 27, 39, 53	18 (1%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	PHE	5.4
1	A	88	ALA	5.0
1	D	88	ALA	4.8
1	C	22	SER	4.7
1	C	144	GLY	4.5
1	C	186	VAL	4.3
1	C	188	ALA	4.1
1	C	121	ARG	4.0
1	B	109	PHE	4.0
1	C	25	LEU	3.9
1	B	108	LEU	3.8
1	C	169	ALA	3.7
1	D	90	GLY	3.6
1	B	163	GLY	3.6
1	F	83	GLY	3.5
1	F	76	TRP	3.4
1	F	8	LEU	3.4
1	B	73	GLY	3.4
1	D	87	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	180	ALA	3.3
1	F	103	GLY	3.2
1	B	123	ILE	3.2
1	C	136	TRP	3.1
1	C	185	ALA	3.1
1	C	163	GLY	3.0
1	E	88	ALA	3.0
1	B	115	LEU	3.0
1	D	71	ALA	3.0
1	C	88	ALA	2.9
1	F	89	LEU	2.9
1	B	71	ALA	2.9
1	C	27	ASP	2.9
1	C	138	TYR	2.9
1	F	88	ALA	2.9
1	C	122	HIS	2.9
1	F	87	THR	2.9
1	C	21	TRP	2.9
1	B	145	PRO	2.8
1	D	5	GLU	2.8
1	B	87	THR	2.8
1	D	84	ARG	2.8
1	B	90	GLY	2.8
1	C	11	ALA	2.8
1	B	144	GLY	2.8
1	F	124	GLY	2.8
1	A	87	THR	2.7
1	F	59	GLY	2.7
1	C	85	GLU	2.7
1	F	99	ASP	2.7
1	B	139	GLN	2.6
1	A	166	ALA	2.6
1	C	133	ALA	2.6
1	C	128	VAL	2.6
1	F	58	THR	2.6
1	C	26	PRO	2.6
1	F	60	TYR	2.6
1	B	147	THR	2.6
1	F	102	THR	2.6
1	D	98	LEU	2.6
1	A	94	CYS	2.6
1	C	191	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	187	PHE	2.5
1	C	67	VAL	2.5
1	B	94	CYS	2.5
1	D	93	LEU	2.5
1	B	114	VAL	2.5
1	D	141	PRO	2.5
1	B	70	ALA	2.5
1	C	141	PRO	2.5
1	F	126	ARG	2.5
1	D	59	GLY	2.5
1	B	136	TRP	2.5
1	A	167	SER	2.4
1	D	153	ALA	2.4
1	E	166	ALA	2.4
1	C	155	GLY	2.4
1	C	139	GLN	2.4
1	A	27	ASP	2.4
1	C	76	TRP	2.4
1	C	24	MET	2.4
1	C	106	ALA	2.4
1	F	153	ALA	2.4
1	C	43	ILE	2.4
1	C	178	SER	2.4
1	B	74	ARG	2.4
1	C	190	LYS	2.4
1	C	23	PRO	2.4
1	F	189	ALA	2.3
1	C	29	GLN	2.3
1	E	25	LEU	2.3
1	C	45	ARG	2.3
1	F	131	ARG	2.3
1	C	50	PHE	2.3
1	C	147	THR	2.3
1	F	94	CYS	2.3
1	B	27	ASP	2.3
1	C	108	LEU	2.3
1	C	170	SER	2.2
1	B	52	PRO	2.2
1	D	26	PRO	2.2
1	A	86	ARG	2.2
1	A	191	ARG	2.2
1	D	81	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	90	GLY	2.2
1	F	93	LEU	2.2
1	C	12	ARG	2.2
1	C	182	ILE	2.2
1	F	122	HIS	2.2
1	C	143	LYS	2.2
1	B	103	GLY	2.1
1	C	119	GLY	2.1
1	C	135	GLY	2.1
1	D	106	ALA	2.1
1	A	4	ARG	2.1
1	F	125	ARG	2.1
1	F	53	TRP	2.1
1	F	74	ARG	2.1
1	C	71	ALA	2.1
1	E	89	LEU	2.1
1	F	98	LEU	2.1
1	F	143	LYS	2.1
1	B	161	VAL	2.1
1	C	70	ALA	2.1
1	C	65	SER	2.1
1	C	94[A]	CYS	2.1
1	C	80	VAL	2.1
1	E	189	ALA	2.1
1	F	85	GLU	2.0
1	F	180	ALA	2.1
1	E	57	ASP	2.0
1	E	99	ASP	2.0
1	A	190	LYS	2.0
1	E	27	ASP	2.0
1	E	121	ARG	2.0
1	B	124	GLY	2.0
1	E	90	GLY	2.0
1	F	155	GLY	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 [i](#)

There are no oligosaccharides 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.