



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 11:56 PM UTC

PDB ID : 4BJN / pdb_00004bjn
Title : Crystal structure of the flax-rust effector AvrM-A
Authors : Ve, T.; Williams, S.J.; Kobe, B.
Deposited on : 2013-04-19
Resolution : 2.90 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

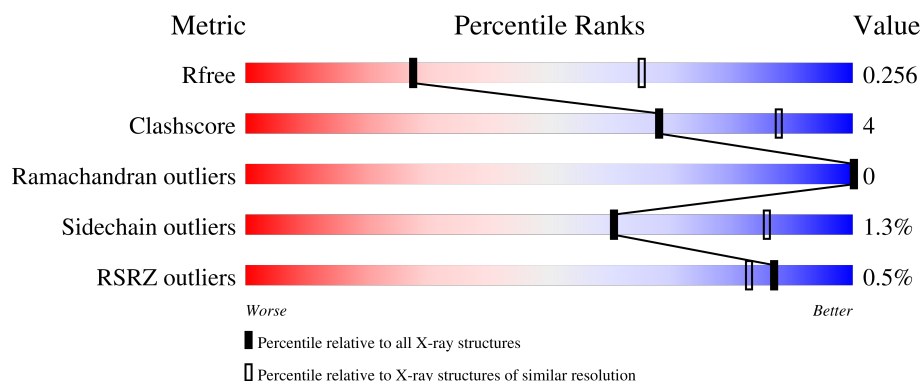
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	244	82% 9% 9%
1	B	244	76% 14% 10%
1	C	244	76% 10% 14%
1	D	244	74% 9% 17%
1	E	244	77% 14% 9%

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Mol	Chain	Length	Quality of chain
1	F	244	 76%7% • 16%
1	G	244	 78%13% • 9%
1	H	244	 78%10% • 11%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 13996 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 AVR-M-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1804	1138	315	348	3			
1	B	219	Total	C	N	O	S	0	0	0
			1783	1126	313	341	3			
1	C	211	Total	C	N	O	S	0	0	0
			1717	1090	298	326	3			
1	D	203	Total	C	N	O	S	0	0	0
			1647	1042	286	316	3			
1	E	222	Total	C	N	O	S	0	0	0
			1803	1137	316	347	3			
1	F	206	Total	C	N	O	S	0	0	0
			1678	1063	293	319	3			
1	G	223	Total	C	N	O	S	0	0	0
			1809	1145	315	346	3			
1	H	216	Total	C	N	O	S	0	0	0
			1755	1108	307	337	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	SER	-	expression tag	UNP Q2MV52
A	101	ASN	-	expression tag	UNP Q2MV52
A	102	ALA	-	expression tag	UNP Q2MV52
B	100	SER	-	expression tag	UNP Q2MV52
B	101	ASN	-	expression tag	UNP Q2MV52
B	102	ALA	-	expression tag	UNP Q2MV52
C	100	SER	-	expression tag	UNP Q2MV52
C	101	ASN	-	expression tag	UNP Q2MV52
C	102	ALA	-	expression tag	UNP Q2MV52
D	100	SER	-	expression tag	UNP Q2MV52
D	101	ASN	-	expression tag	UNP Q2MV52
D	102	ALA	-	expression tag	UNP Q2MV52
E	100	SER	-	expression tag	UNP Q2MV52

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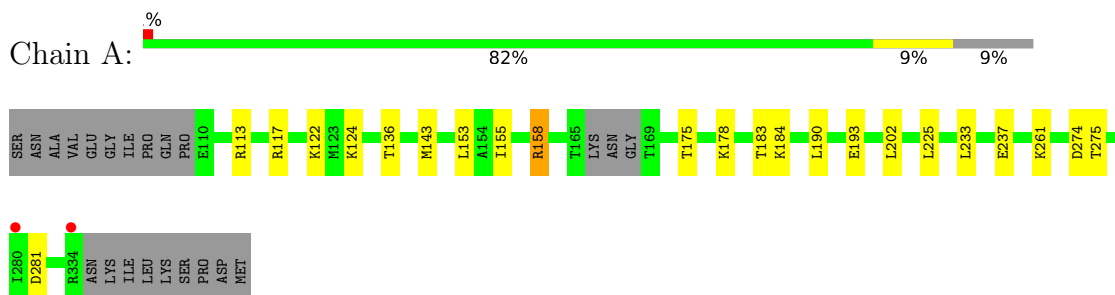
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Chain	Residue	Modelled	Actual	Comment	Reference
E	101	ASN	-	expression tag	UNP Q2MV52
E	102	ALA	-	expression tag	UNP Q2MV52
F	100	SER	-	expression tag	UNP Q2MV52
F	101	ASN	-	expression tag	UNP Q2MV52
F	102	ALA	-	expression tag	UNP Q2MV52
G	100	SER	-	expression tag	UNP Q2MV52
G	101	ASN	-	expression tag	UNP Q2MV52
G	102	ALA	-	expression tag	UNP Q2MV52
H	100	SER	-	expression tag	UNP Q2MV52
H	101	ASN	-	expression tag	UNP Q2MV52
H	102	ALA	-	expression tag	UNP Q2MV52

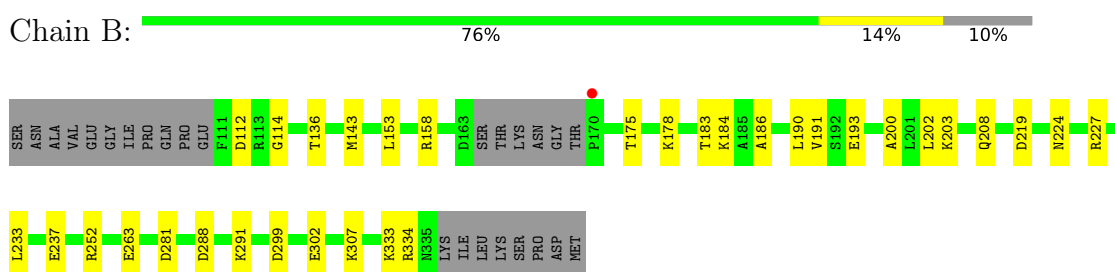
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

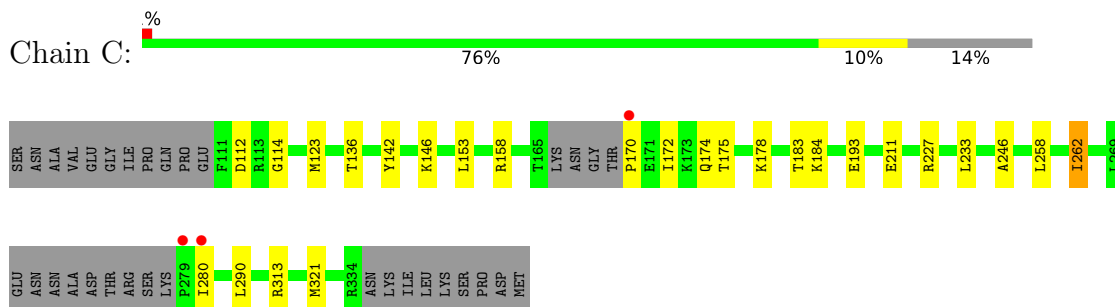
• Molecule 1: AVRMA-A



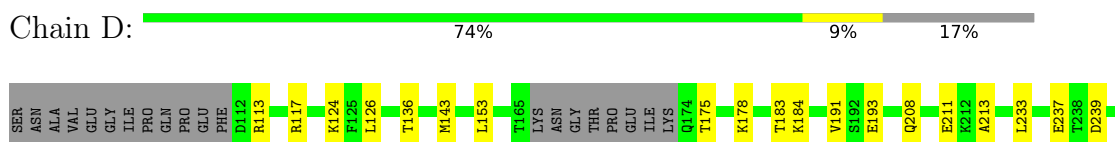
• Molecule 1: AVRMA-A

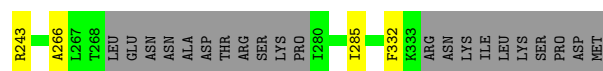


• Molecule 1: AVRMA-A



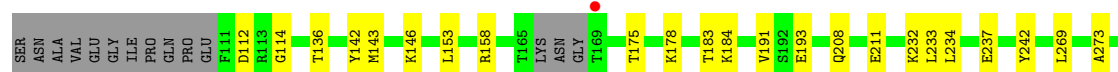
• Molecule 1: AVRMA-A





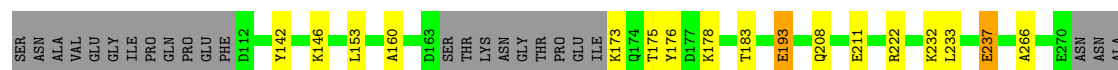
• Molecule 1: AVR-M-A

Chain E: 77% 14% 9%



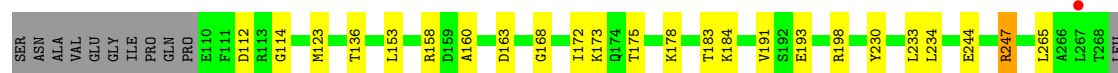
• Molecule 1: AVR-M-A

Chain F: 76% 7% 16%



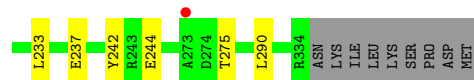
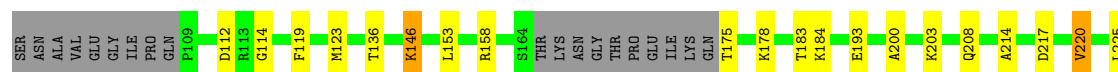
• Molecule 1: AVR-M-A

Chain G: 78% 13% 9%



• Molecule 1: AVR-M-A

Chain H: 78% 10% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	116.99Å 131.39Å 280.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 2.90 49.59 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.59-2.90) 99.8 (49.59-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.207 , 0.249 0.220 , 0.256	Depositor DCC
R_{free} test set	2438 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13996	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

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	0.78	0/1826	1.41	8/2449 (0.3%)
1	B	0.79	0/1805	1.41	8/2419 (0.3%)
1	C	0.80	0/1738	1.41	8/2327 (0.3%)
1	D	0.78	0/1665	1.39	4/2230 (0.2%)
1	E	0.80	0/1825	1.38	5/2448 (0.2%)
1	F	0.74	0/1697	1.41	11/2271 (0.5%)
1	G	0.85	1/1832 (0.1%)	1.45	13/2455 (0.5%)
1	H	0.80	0/1777	1.38	4/2382 (0.2%)
All	All	0.79	1/14165 (0.0%)	1.41	61/18981 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	123	MET	SD-CE	-6.03	1.64	1.79

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	LEU	CA-C-N	6.80	129.28	120.44
1	C	233	LEU	C-N-CA	6.80	129.28	120.44
1	F	237	GLU	CB-CG-CD	6.51	123.67	112.60
1	G	233	LEU	CA-C-N	6.47	128.85	120.44
1	G	233	LEU	C-N-CA	6.47	128.85	120.44
1	E	193	GLU	CA-C-N	6.15	128.52	120.28
1	E	193	GLU	C-N-CA	6.15	128.52	120.28
1	H	193	GLU	CA-C-N	6.03	128.35	120.28
1	H	193	GLU	C-N-CA	6.03	128.35	120.28
1	B	281	ASP	CA-CB-CG	6.02	118.62	112.60
1	C	280	ILE	CA-C-N	6.01	129.66	120.82
1	C	280	ILE	C-N-CA	6.01	129.66	120.82
1	B	193	GLU	CA-C-N	6.00	128.31	120.28
1	B	193	GLU	C-N-CA	6.00	128.31	120.28
1	F	193	GLU	CA-C-N	5.99	128.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	193	GLU	C-N-CA	5.99	128.31	120.28
1	G	336	LYS	CA-C-N	5.97	130.36	121.77
1	G	336	LYS	C-N-CA	5.97	130.36	121.77
1	A	274	ASP	CA-CB-CG	5.96	118.56	112.60
1	D	193	GLU	CA-C-N	5.95	128.25	120.28
1	D	193	GLU	C-N-CA	5.95	128.25	120.28
1	G	193	GLU	CA-C-N	5.91	128.20	120.28
1	G	193	GLU	C-N-CA	5.91	128.20	120.28
1	C	193	GLU	CA-C-N	5.87	128.14	120.28
1	C	193	GLU	C-N-CA	5.87	128.14	120.28
1	C	262	ILE	CA-C-N	5.82	128.08	120.28
1	C	262	ILE	C-N-CA	5.82	128.08	120.28
1	G	168	GLY	CA-C-N	5.71	126.85	120.06
1	G	168	GLY	C-N-CA	5.71	126.85	120.06
1	F	160	ALA	CA-C-N	5.70	127.85	120.44
1	F	160	ALA	C-N-CA	5.70	127.85	120.44
1	A	281	ASP	CA-CB-CG	5.61	118.21	112.60
1	G	160	ALA	CA-C-N	5.61	128.25	120.29
1	G	160	ALA	C-N-CA	5.61	128.25	120.29
1	A	193	GLU	CA-C-N	5.59	127.78	120.28
1	A	193	GLU	C-N-CA	5.59	127.78	120.28
1	B	263	GLU	CB-CG-CD	5.41	121.80	112.60
1	G	337	ILE	N-CA-CB	-5.38	103.89	112.07
1	A	275	THR	CA-C-N	5.38	127.75	120.38
1	A	275	THR	C-N-CA	5.38	127.75	120.38
1	B	333	LYS	CA-C-N	5.38	129.29	120.63
1	B	333	LYS	C-N-CA	5.38	129.29	120.63
1	G	247	ARG	CA-C-N	5.35	127.78	120.46
1	G	247	ARG	C-N-CA	5.35	127.78	120.46
1	E	335	ASN	CA-CB-CG	5.26	117.86	112.60
1	H	208	GLN	CA-C-N	5.21	127.22	120.44
1	H	208	GLN	C-N-CA	5.21	127.22	120.44
1	D	208	GLN	CA-C-N	5.21	127.21	120.44
1	D	208	GLN	C-N-CA	5.21	127.21	120.44
1	B	208	GLN	CA-C-N	5.18	127.17	120.44
1	B	208	GLN	C-N-CA	5.18	127.17	120.44
1	A	274	ASP	CA-C-N	5.14	127.44	120.65
1	A	274	ASP	C-N-CA	5.14	127.44	120.65
1	F	208	GLN	CA-C-N	5.12	127.09	120.44
1	F	208	GLN	C-N-CA	5.12	127.09	120.44
1	F	232	LYS	CA-C-N	5.10	127.11	120.28
1	F	232	LYS	C-N-CA	5.10	127.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	306	TYR	CA-C-N	5.03	127.02	120.28
1	F	306	TYR	C-N-CA	5.03	127.02	120.28
1	E	208	GLN	CA-C-N	5.03	126.98	120.44
1	E	208	GLN	C-N-CA	5.03	126.98	120.44

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	1804	0	1847	14	0
1	B	1783	0	1829	17	0
1	C	1717	0	1770	13	0
1	D	1647	0	1691	10	0
1	E	1803	0	1847	21	0
1	F	1678	0	1730	9	0
1	G	1809	0	1864	16	0
1	H	1755	0	1796	19	0
All	All	13996	0	14374	103	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 4.

All (103) 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:G:335:ASN:HA	1:G:338:LEU:HD13	1.49	0.93
1:D:153:LEU:HB3	1:D:183:THR:HG22	1.66	0.77
1:B:153:LEU:HB3	1:B:183:THR:HG22	1.65	0.77
1:A:153:LEU:HB3	1:A:183:THR:HG22	1.67	0.77
1:F:153:LEU:HB3	1:F:183:THR:HG22	1.67	0.76
1:C:153:LEU:HB3	1:C:183:THR:HG22	1.68	0.76
1:H:153:LEU:HB3	1:H:183:THR:HG22	1.67	0.76
1:G:153:LEU:HB3	1:G:183:THR:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LEU:HB3	1:E:183:THR:HG22	1.67	0.75
1:E:143:MET:CE	1:E:191:VAL:HG13	2.21	0.70
1:G:163:ASP:HB2	1:G:172:ILE:HG21	1.74	0.69
1:F:193:GLU:HB2	1:G:173:LYS:HE2	1.75	0.68
1:E:237:GLU:HG2	1:H:233:LEU:HD22	1.76	0.66
1:B:143:MET:CE	1:B:191:VAL:HG13	2.27	0.64
1:E:233:LEU:HD22	1:H:237:GLU:HG2	1.81	0.62
1:G:230:TYR:O	1:G:234:LEU:HB2	2.00	0.62
1:C:123:MET:HE2	1:C:146:LYS:HD3	1.82	0.61
1:A:233:LEU:HD22	1:B:237:GLU:HG2	1.84	0.59
1:D:239:ASP:O	1:D:243:ARG:HG2	2.05	0.57
1:D:266:ALA:HA	1:D:285:ILE:HD12	1.86	0.57
1:C:258:LEU:O	1:C:262:ILE:HG12	2.07	0.55
1:A:113:ARG:HA	1:A:158:ARG:HH11	1.71	0.55
1:A:117:ARG:HH22	1:A:124:LYS:HD2	1.71	0.55
1:E:114:GLY:H	1:E:158:ARG:HD3	1.72	0.55
1:G:293:GLN:HA	1:G:296:LEU:HD12	1.90	0.54
1:G:198:ARG:HG2	1:G:334:ARG:HA	1.89	0.53
1:F:266:ALA:HA	1:F:285:ILE:HD12	1.92	0.52
1:C:123:MET:CE	1:C:146:LYS:HD3	2.39	0.52
1:F:323:GLU:HG3	1:H:275:THR:HG21	1.92	0.52
1:A:237:GLU:HG2	1:B:233:LEU:HD22	1.92	0.52
1:C:227:ARG:HD3	1:C:321:MET:SD	2.49	0.52
1:H:123:MET:HE2	1:H:146:LYS:HD3	1.92	0.52
1:H:242:TYR:HA	1:H:290:LEU:HD21	1.93	0.51
1:E:143:MET:HE3	1:E:191:VAL:HG13	1.92	0.50
1:F:173:LYS:HA	1:F:176:TYR:HB3	1.93	0.49
1:F:233:LEU:O	1:F:237:GLU:HG3	2.13	0.49
1:C:174:GLN:HG2	1:C:178:LYS:HE3	1.94	0.48
1:H:214:ALA:HA	1:H:220:VAL:HG23	1.95	0.48
1:E:273:ALA:HB2	1:E:280:ILE:HD11	1.95	0.47
1:E:142:TYR:CZ	1:E:146:LYS:HE2	2.50	0.47
1:C:170:PRO:HD2	1:C:172:ILE:HG12	1.97	0.47
1:E:293:GLN:HE21	1:H:119:PHE:HE2	1.62	0.47
1:G:198:ARG:CB	1:G:337:ILE:HG13	2.44	0.47
1:B:224:ASN:HD21	1:B:227:ARG:HH21	1.62	0.47
1:F:222:ARG:HH12	1:H:275:THR:HA	1.80	0.47
1:B:186:ALA:O	1:B:190:LEU:HG	2.15	0.47
1:C:112:ASP:O	1:C:158:ARG:HD2	2.15	0.47
1:H:217:ASP:HB3	1:H:220:VAL:HG22	1.97	0.47
1:D:143:MET:CE	1:D:191:VAL:HG13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:ASP:O	1:G:158:ARG:HD2	2.16	0.46
1:E:112:ASP:O	1:E:158:ARG:HD2	2.16	0.45
1:D:175:THR:HA	1:D:178:LYS:HD2	1.97	0.45
1:E:290:LEU:HD23	1:E:310:ILE:HD11	1.98	0.45
1:C:175:THR:HA	1:C:178:LYS:HD2	1.99	0.45
1:D:124:LYS:HE2	1:D:126:LEU:HD21	1.98	0.45
1:C:114:GLY:H	1:C:158:ARG:HD3	1.82	0.45
1:F:175:THR:HA	1:F:178:LYS:HD2	1.98	0.45
1:H:112:ASP:O	1:H:158:ARG:HD2	2.17	0.44
1:H:123:MET:CE	1:H:146:LYS:HD3	2.47	0.44
1:A:155:ILE:HG12	1:A:158:ARG:NH2	2.32	0.44
1:B:112:ASP:O	1:B:158:ARG:HD2	2.17	0.44
1:G:198:ARG:HB3	1:G:337:ILE:HG13	1.99	0.44
1:H:114:GLY:H	1:H:158:ARG:HD3	1.82	0.44
1:G:175:THR:HA	1:G:178:LYS:HD2	2.00	0.44
1:E:302:GLU:HA	1:H:225:LEU:HD21	2.00	0.44
1:E:269:LEU:HB3	1:E:280:ILE:HG12	2.00	0.44
1:A:175:THR:HA	1:A:178:LYS:HD2	1.99	0.44
1:F:142:TYR:CZ	1:F:146:LYS:HE2	2.52	0.44
1:B:136:THR:HG21	1:B:184:LYS:HE3	2.00	0.44
1:G:136:THR:HG21	1:G:184:LYS:HE3	1.99	0.44
1:H:175:THR:HA	1:H:178:LYS:HD2	1.99	0.43
1:E:136:THR:HG21	1:E:184:LYS:HE3	2.00	0.43
1:C:136:THR:HG21	1:C:184:LYS:HE3	2.01	0.43
1:A:122:LYS:HG3	1:B:299:ASP:HB3	2.00	0.43
1:B:175:THR:HA	1:B:178:LYS:HD2	1.99	0.43
1:B:114:GLY:H	1:B:158:ARG:HD3	1.84	0.43
1:B:291:LYS:HG2	1:B:307:LYS:HG3	2.01	0.43
1:B:202:LEU:HA	1:B:334:ARG:HD2	2.00	0.42
1:D:233:LEU:O	1:D:237:GLU:HG3	2.19	0.42
1:H:136:THR:HG21	1:H:184:LYS:HE3	2.01	0.42
1:G:114:GLY:H	1:G:158:ARG:HD3	1.84	0.42
1:C:142:TYR:CZ	1:C:146:LYS:HE2	2.54	0.42
1:A:143:MET:HE2	1:A:190:LEU:HD13	2.00	0.42
1:E:232:LYS:HE2	1:H:244:GLU:OE2	2.19	0.42
1:C:246:ALA:HA	1:C:290:LEU:HD22	2.01	0.42
1:A:155:ILE:HG12	1:A:158:ARG:HH21	1.84	0.42
1:E:290:LEU:HD23	1:E:310:ILE:CD1	2.50	0.41
1:D:136:THR:HG21	1:D:184:LYS:HE3	2.01	0.41
1:A:113:ARG:HD3	1:B:252:ARG:O	2.21	0.41
1:E:234:LEU:HG	1:E:283:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:GLU:OE1	1:G:247:ARG:NH1	2.54	0.41
1:A:202:LEU:HD11	1:D:117:ARG:NH1	2.35	0.41
1:E:242:TYR:HA	1:E:290:LEU:HD11	2.02	0.41
1:B:224:ASN:ND2	1:B:227:ARG:HH21	2.18	0.41
1:A:225:LEU:HD21	1:B:302:GLU:HA	2.02	0.41
1:E:175:THR:HA	1:E:178:LYS:HD2	2.02	0.41
1:E:302:GLU:HG3	1:H:225:LEU:HD11	2.03	0.41
1:A:136:THR:HG21	1:A:184:LYS:HE3	2.02	0.40
1:E:298:ALA:HB2	1:G:337:ILE:HD12	2.03	0.40
1:H:200:ALA:HA	1:H:203:LYS:HD2	2.03	0.40
1:G:300:ASP:HB3	1:G:303:LEU:HB2	2.02	0.40
1:B:200:ALA:HA	1:B:203:LYS:HD2	2.03	0.40
1:D:213:ALA:HB2	1:D:332:PHE:HE2	1.86	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	218/244 (89%)	212 (97%)	6 (3%)	0	100	100
1	B	215/244 (88%)	212 (99%)	3 (1%)	0	100	100
1	C	205/244 (84%)	201 (98%)	4 (2%)	0	100	100
1	D	197/244 (81%)	194 (98%)	3 (2%)	0	100	100
1	E	218/244 (89%)	215 (99%)	3 (1%)	0	100	100
1	F	200/244 (82%)	196 (98%)	4 (2%)	0	100	100
1	G	219/244 (90%)	215 (98%)	4 (2%)	0	100	100
1	H	212/244 (87%)	207 (98%)	5 (2%)	0	100	100
All	All	1684/1952 (86%)	1652 (98%)	32 (2%)	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	190/209 (91%)	188 (99%)	2 (1%)	65	88
1	B	187/209 (90%)	185 (99%)	2 (1%)	65	88
1	C	180/209 (86%)	178 (99%)	2 (1%)	65	88
1	D	172/209 (82%)	170 (99%)	2 (1%)	63	86
1	E	190/209 (91%)	185 (97%)	5 (3%)	40	73
1	F	175/209 (84%)	174 (99%)	1 (1%)	78	93
1	G	191/209 (91%)	188 (98%)	3 (2%)	55	83
1	H	184/209 (88%)	182 (99%)	2 (1%)	65	88
All	All	1469/1672 (88%)	1450 (99%)	19 (1%)	61	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	261	LYS
1	B	219	ASP
1	B	288	ASP
1	C	211	GLU
1	C	313	ARG
1	D	113	ARG
1	D	211	GLU
1	E	211	GLU
1	E	288	ASP
1	E	290	LEU
1	E	323	GLU
1	E	334	ARG
1	F	211	GLU
1	G	191	VAL
1	G	265	LEU

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Mol	Chain	Res	Type
1	G	337	ILE
1	H	146	LYS
1	H	220	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	272	ASN
1	B	224	ASN
1	B	293	GLN
1	C	174	GLN
1	C	293	GLN
1	E	174	GLN
1	E	293	GLN
1	E	297	HIS
1	E	335	ASN
1	F	293	GLN
1	G	295	ASN
1	G	335	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	222/244 (90%)	-0.01	2 (0%) 81 75	54, 101, 167, 188	0
1	B	219/244 (89%)	-0.21	1 (0%) 87 83	50, 93, 154, 188	0
1	C	211/244 (86%)	-0.25	3 (1%) 73 65	41, 78, 154, 185	0
1	D	203/244 (83%)	-0.18	0 100 100	45, 96, 149, 185	0
1	E	222/244 (90%)	-0.36	1 (0%) 87 83	46, 76, 125, 173	0
1	F	206/244 (84%)	-0.11	0 100 100	59, 100, 159, 203	0
1	G	223/244 (91%)	-0.11	1 (0%) 88 85	48, 84, 175, 200	0
1	H	216/244 (88%)	0.00	1 (0%) 87 83	50, 95, 164, 186	0
All	All	1722/1952 (88%)	-0.15	9 (0%) 87 83	41, 90, 159, 203	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	PRO	3.6
1	G	267	LEU	2.7
1	C	279	PRO	2.4
1	A	280	ILE	2.3
1	A	334	ARG	2.3
1	B	170	PRO	2.3
1	E	169	THR	2.1
1	H	273	ALA	2.1
1	C	280	ILE	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 [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.