



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:10 PM UTC

PDB ID : 1SMV / pdb_00001smv
Title : PRIMARY STRUCTURE OF SESBANIA MOSAIC VIRUS COAT PROTEIN: ITS IMPLICATIONS TO THE ASSEMBLY AND ARCHITECTURE OF THE VIRUS
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Deposited on : 1995-06-16
Resolution : 3.00 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

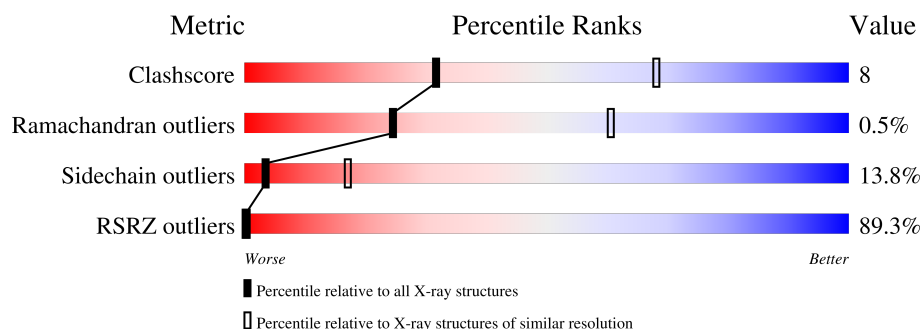
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	266	65% 52% 18% • 26%
1	B	266	65% 55% 14% • • 26%
1	C	266	76% 65% 14% • • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4516 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 SESBANIA MOSAIC VIRUS COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1437	911	234	284	8			
1	B	196	Total	C	N	O	S	0	0	0
			1452	924	234	287	7			
1	C	222	Total	C	N	O	S	0	0	0
			1623	1028	269	316	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ILE	LYS	conflict	UNP Q9EB06
A	36	PRO	GLN	conflict	UNP Q9EB06
A	38	ILE	THR	conflict	UNP Q9EB06
A	66	ALA	GLY	conflict	UNP Q9EB06
A	?	-	THR	deletion	UNP Q9EB06
A	72	CYS	SER	conflict	UNP Q9EB06
A	75	THR	SER	conflict	UNP Q9EB06
A	105	ASP	ALA	conflict	UNP Q9EB06
A	149	LYS	GLN	conflict	UNP Q9EB06
A	173	ASN	GLY	conflict	UNP Q9EB06
A	174	SER	THR	conflict	UNP Q9EB06
A	191	GLU	LYS	conflict	UNP Q9EB06
A	218	ASP	PRO	conflict	UNP Q9EB06
A	244	ASP	CYS	conflict	UNP Q9EB06
B	0	ILE	LYS	conflict	UNP Q9EB06
B	36	PRO	GLN	conflict	UNP Q9EB06
B	38	ILE	THR	conflict	UNP Q9EB06
B	66	ALA	GLY	conflict	UNP Q9EB06
B	?	-	THR	deletion	UNP Q9EB06
B	72	CYS	SER	conflict	UNP Q9EB06
B	75	THR	SER	conflict	UNP Q9EB06
B	105	ASP	ALA	conflict	UNP Q9EB06
B	149	LYS	GLN	conflict	UNP Q9EB06

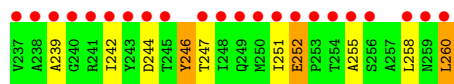
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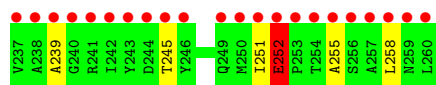
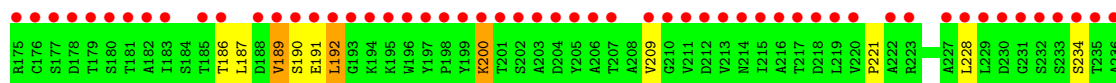
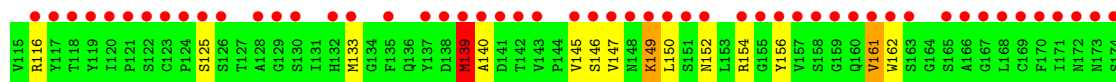
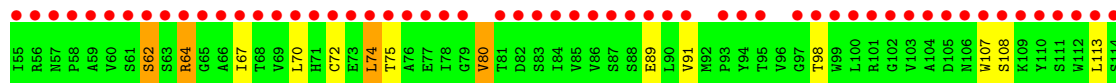
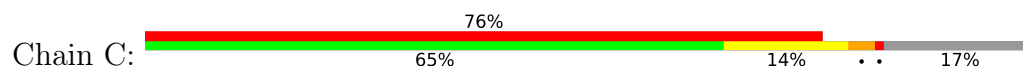
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	ASN	GLY	conflict	UNP Q9EB06
B	174	SER	THR	conflict	UNP Q9EB06
B	191	GLU	LYS	conflict	UNP Q9EB06
B	218	ASP	PRO	conflict	UNP Q9EB06
B	244	ASP	CYS	conflict	UNP Q9EB06
C	0	ILE	LYS	conflict	UNP Q9EB06
C	36	PRO	GLN	conflict	UNP Q9EB06
C	38	ILE	THR	conflict	UNP Q9EB06
C	66	ALA	GLY	conflict	UNP Q9EB06
C	?	-	THR	deletion	UNP Q9EB06
C	72	CYS	SER	conflict	UNP Q9EB06
C	75	THR	SER	conflict	UNP Q9EB06
C	105	ASP	ALA	conflict	UNP Q9EB06
C	149	LYS	GLN	conflict	UNP Q9EB06
C	173	ASN	GLY	conflict	UNP Q9EB06
C	174	SER	THR	conflict	UNP Q9EB06
C	191	GLU	LYS	conflict	UNP Q9EB06
C	218	ASP	PRO	conflict	UNP Q9EB06
C	244	ASP	CYS	conflict	UNP Q9EB06

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Ca 3 3	0	0
2	C	1	Total Ca 1 1	0	0



● Molecule 1: SESBANIA MOSAIC VIRUS COAT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	R 3	Depositor
Cell constants a, b, c, α , β , γ	291.46Å 291.46Å 291.46Å 61.95° 61.95° 61.95°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	70.0 (10.00-3.00) 68.2 (10.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.227 , (Not available) 0.700 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.76 , 129.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.17	EDS
Total number of atoms	4516	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.85	2/1468 (0.1%)	1.18	17/2012 (0.8%)
1	B	0.75	1/1483 (0.1%)	1.11	12/2033 (0.6%)
1	C	0.79	1/1656 (0.1%)	1.09	9/2268 (0.4%)
All	All	0.80	4/4607 (0.1%)	1.13	38/6313 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	MET	SD-CE	-8.70	1.57	1.79
1	C	139	MET	SD-CE	-6.28	1.63	1.79
1	A	69	VAL	CA-CB	6.00	1.63	1.54
1	B	69	VAL	CA-CB	5.82	1.62	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ILE	N-CA-C	7.45	119.21	108.48
1	B	255	ALA	N-CA-C	-7.37	99.37	110.28
1	C	234	SER	N-CA-C	-7.09	104.10	112.89
1	C	252	GLU	CA-C-N	7.08	127.11	119.89
1	C	252	GLU	C-N-CA	7.08	127.11	119.89
1	A	113	LEU	N-CA-C	-6.88	105.01	113.41
1	A	259	ASN	N-CA-C	6.84	119.28	108.67
1	A	120	ILE	CA-C-N	6.70	126.67	120.03
1	A	120	ILE	C-N-CA	6.70	126.67	120.03
1	A	211	VAL	N-CA-C	-6.48	104.85	110.74
1	B	219	LEU	N-CA-C	6.40	121.22	113.41
1	A	236	ALA	N-CA-C	6.31	119.51	110.24
1	B	78	ILE	N-CA-C	6.30	116.99	108.17
1	A	219	LEU	N-CA-C	6.22	121.53	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	VAL	N-CA-C	5.96	121.73	109.34
1	A	247	THR	N-CA-C	-5.95	98.16	108.69
1	A	255	ALA	N-CA-C	-5.92	101.07	109.96
1	C	74	LEU	N-CA-C	-5.92	101.07	109.96
1	C	189	VAL	N-CA-C	5.91	119.33	111.17
1	A	234	SER	N-CA-C	-5.86	106.09	113.18
1	B	160	GLN	CA-CB-CG	-5.69	102.71	114.10
1	B	247	THR	N-CA-C	-5.68	99.16	108.76
1	B	213	VAL	CB-CA-C	-5.68	103.76	112.05
1	A	252	GLU	CA-C-N	5.65	126.90	119.84
1	A	252	GLU	C-N-CA	5.65	126.90	119.84
1	C	108	SER	N-CA-C	5.61	117.48	111.36
1	B	246	TYR	N-CA-C	5.50	118.05	109.52
1	B	194	LYS	N-CA-CB	-5.48	103.23	111.56
1	C	255	ALA	N-CA-C	-5.45	102.33	110.23
1	C	80	VAL	CB-CA-C	-5.42	103.44	111.19
1	A	98	THR	N-CA-C	5.42	116.87	111.07
1	B	192	LEU	N-CA-C	-5.37	103.45	110.53
1	B	70	LEU	CA-CB-CG	-5.36	97.56	116.30
1	A	70	LEU	N-CA-C	-5.25	100.35	108.90
1	A	178	ASP	CA-C-N	-5.14	114.42	122.65
1	A	178	ASP	C-N-CA	-5.14	114.42	122.65
1	C	64	ARG	N-CA-C	5.09	117.45	107.57
1	B	98	THR	N-CA-C	5.03	117.65	111.82

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	1437	0	1369	25	0
1	B	1452	0	1416	26	0
1	C	1623	0	1586	28	0
2	A	3	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4516	0	4371	72	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 8.

All (72) 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:145:VAL:HG23	1:A:149:LYS:HE3	1.42	1.00
1:A:72:CYS:SG	1:A:245:THR:HG23	2.08	0.93
1:A:149:LYS:HD3	1:B:258:LEU:HD21	1.47	0.92
1:B:116:ARG:HB2	1:B:186:THR:HG22	1.52	0.91
1:C:72:CYS:SG	1:C:245:THR:HG23	2.16	0.85
1:C:145:VAL:H	1:C:149:LYS:HE2	1.44	0.83
1:C:145:VAL:HG22	1:C:149:LYS:HE2	1.64	0.78
1:A:104:ALA:HA	1:A:250:MET:CE	2.21	0.71
1:A:145:VAL:H	1:A:149:LYS:HD2	1.56	0.70
1:A:75:THR:HG22	1:A:242:ILE:O	1.92	0.70
1:C:67:ILE:HD13	1:C:107:TRP:HE1	1.57	0.70
1:C:139:MET:HE3	1:C:139:MET:HA	1.74	0.67
1:B:172:ASN:H	1:B:172:ASN:HD22	1.44	0.66
1:A:104:ALA:HA	1:A:250:MET:HE2	1.77	0.65
1:C:62:SER:HB3	1:C:67:ILE:HG13	1.80	0.64
1:B:189:VAL:HA	1:B:192:LEU:HD22	1.80	0.62
1:C:161:VAL:HG22	1:C:239:ALA:HB1	1.81	0.62
1:B:75:THR:HG22	1:B:242:ILE:O	1.99	0.62
1:C:133:MET:O	1:C:156:TYR:HA	2.00	0.60
1:A:161:VAL:HG22	1:A:239:ALA:HB1	1.85	0.58
1:C:116:ARG:HB2	1:C:186:THR:HG22	1.86	0.57
1:A:258:LEU:HD21	1:C:149:LYS:HZ1	1.69	0.57
1:A:260:LEU:HD23	1:C:140:ALA:O	2.05	0.57
1:A:77:GLU:HG2	1:A:241:ARG:HG2	1.87	0.57
1:C:251:ILE:HG13	1:C:252:GLU:HG2	1.87	0.56
1:A:72:CYS:SG	1:A:245:THR:CG2	2.90	0.55
1:A:151:SER:HA	1:A:156:TYR:CD1	2.41	0.54
1:C:67:ILE:HD13	1:C:107:TRP:NE1	2.21	0.53
1:A:244:ASP:OD1	1:A:246:TYR:HD2	1.90	0.53
1:B:251:ILE:HG13	1:B:252:GLU:HG2	1.90	0.53
1:A:258:LEU:HD21	1:C:149:LYS:NZ	2.23	0.53
1:B:229:LEU:HD23	1:B:229:LEU:N	2.24	0.52
1:C:154:ARG:HH11	1:C:154:ARG:HG2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:VAL:H	1:C:149:LYS:CE	2.20	0.51
1:B:109:LYS:HE2	1:B:252:GLU:OE2	2.11	0.51
1:B:172:ASN:HD22	1:B:172:ASN:N	2.06	0.50
1:A:144:PRO:HA	1:A:149:LYS:HD2	1.93	0.50
1:C:189:VAL:HA	1:C:192:LEU:HD22	1.93	0.50
1:C:139:MET:HA	1:C:139:MET:CE	2.42	0.50
1:A:133:MET:O	1:A:156:TYR:HA	2.13	0.48
1:C:139:MET:HE3	1:C:139:MET:CA	2.43	0.48
1:B:145:VAL:HG12	1:B:149:LYS:CE	2.44	0.48
1:C:113:LEU:HD23	1:C:113:LEU:HA	1.67	0.47
1:A:104:ALA:HA	1:A:250:MET:HE1	1.96	0.47
1:B:133:MET:O	1:B:156:TYR:HA	2.14	0.47
1:A:172:ASN:O	1:A:172:ASN:CG	2.58	0.46
1:A:140:ALA:O	1:B:260:LEU:HD12	2.16	0.46
1:C:125:SER:HA	1:C:162:TRP:CG	2.50	0.45
1:B:138:ASP:OD2	1:C:200:LYS:HE3	2.17	0.45
1:B:251:ILE:C	1:B:252:GLU:HG2	2.40	0.45
1:A:154:ARG:CZ	1:A:188:ASP:HB3	2.47	0.45
1:B:67:ILE:HG12	1:B:107:TRP:CZ2	2.52	0.44
1:C:145:VAL:HG22	1:C:149:LYS:CE	2.42	0.44
1:A:166:ALA:HB1	1:A:178:ASP:O	2.16	0.44
1:C:146:SER:OG	1:C:149:LYS:HD3	2.17	0.44
1:B:116:ARG:HB2	1:B:186:THR:CG2	2.37	0.44
1:B:195:LYS:HD2	1:B:196:TRP:CE2	2.53	0.44
1:B:169:CYS:HA	1:B:172:ASN:HD21	1.82	0.43
1:A:75:THR:HG22	1:A:242:ILE:C	2.42	0.43
1:B:81:THR:HG22	1:B:236:ALA:HA	2.01	0.43
1:C:251:ILE:C	1:C:252:GLU:HG2	2.44	0.42
1:B:145:VAL:H	1:B:149:LYS:HD2	1.84	0.42
1:B:84:ILE:HA	1:B:229:LEU:HB3	2.01	0.42
1:A:77:GLU:OE2	1:A:241:ARG:NH1	2.53	0.42
1:B:172:ASN:H	1:B:172:ASN:ND2	2.13	0.42
1:B:244:ASP:OD2	1:B:246:TYR:HD2	2.03	0.42
1:B:161:VAL:HB	1:B:239:ALA:HB1	2.01	0.42
1:C:192:LEU:HG	1:C:221:PRO:HB2	2.03	0.41
1:B:151:SER:HA	1:B:156:TYR:CD1	2.55	0.41
1:C:74:LEU:C	1:C:74:LEU:HD23	2.46	0.41
1:B:146:SER:H	1:B:149:LYS:HD2	1.86	0.40
1:A:253:PRO:HB2	1:C:152:ASN: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	194/266 (73%)	180 (93%)	12 (6%)	2 (1%)	12	45
1	B	194/266 (73%)	184 (95%)	9 (5%)	1 (0%)	24	60
1	C	220/266 (83%)	211 (96%)	9 (4%)	0	100	100
All	All	608/798 (76%)	575 (95%)	30 (5%)	3 (0%)	24	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	B	161	VAL
1	A	189	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	150/220 (68%)	127 (85%)	23 (15%)	3	14
1	B	157/220 (71%)	138 (88%)	19 (12%)	5	21
1	C	172/220 (78%)	148 (86%)	24 (14%)	3	16
All	All	479/660 (73%)	413 (86%)	66 (14%)	3	17

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

Mol	Chain	Res	Type
1	A	72	CYS
1	A	103	VAL
1	A	113	LEU
1	A	116	ARG
1	A	143	VAL
1	A	145	VAL
1	A	150	LEU
1	A	154	ARG
1	A	157	VAL
1	A	161	VAL
1	A	165	SER
1	A	168	LEU
1	A	178	ASP
1	A	186	THR
1	A	189	VAL
1	A	209	VAL
1	A	217	THR
1	A	219	LEU
1	A	225	VAL
1	A	228	LEU
1	A	229	LEU
1	A	232	SER
1	A	260	LEU
1	B	67	ILE
1	B	69	VAL
1	B	70	LEU
1	B	96	VAL
1	B	103	VAL
1	B	145	VAL
1	B	150	LEU
1	B	154	ARG
1	B	165	SER
1	B	172	ASN
1	B	192	LEU
1	B	195	LYS
1	B	213	VAL
1	B	219	LEU
1	B	224	LEU
1	B	228	LEU
1	B	235	THR
1	B	252	GLU
1	B	260	LEU
1	C	43	SER

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Mol	Chain	Res	Type
1	C	52	MET
1	C	62	SER
1	C	64	ARG
1	C	70	LEU
1	C	75	THR
1	C	80	VAL
1	C	89	GLU
1	C	91	VAL
1	C	98	THR
1	C	139	MET
1	C	147	VAL
1	C	149	LYS
1	C	150	LEU
1	C	161	VAL
1	C	187	LEU
1	C	190	SER
1	C	191	GLU
1	C	192	LEU
1	C	200	LYS
1	C	209	VAL
1	C	228	LEU
1	C	252	GLU
1	C	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	172	ASN
1	C	49	GLN
1	C	106	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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	196/266 (73%)	4.71	173 (88%) 0 0	2, 9, 32, 74	0
1	B	196/266 (73%)	4.33	173 (88%) 0 0	3, 10, 33, 58	0
1	C	222/266 (83%)	4.83	202 (90%) 0 0	3, 10, 34, 75	0
All	All	614/798 (76%)	4.63	548 (89%) 0 0	2, 9, 34, 75	0

All (548) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	GLN	24.2
1	A	176	CYS	19.6
1	A	177	SER	19.3
1	A	173	ASN	15.4
1	A	172	ASN	14.3
1	C	126	SER	14.1
1	A	210	GLY	14.1
1	C	62	SER	13.9
1	A	178	ASP	13.0
1	C	180	SER	12.5
1	C	235	THR	12.5
1	C	63	SER	12.2
1	B	65	GLY	12.0
1	C	195	LYS	12.0
1	B	173	ASN	12.0
1	A	97	GLY	11.6
1	C	234	SER	11.5
1	A	76	ALA	11.4
1	A	118	THR	11.1
1	C	174	SER	11.1
1	B	175	ARG	11.0
1	A	65	GLY	11.0
1	B	174	SER	10.6

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Mol	Chain	Res	Type	RSRZ
1	A	235	THR	10.6
1	C	202	SER	10.6
1	A	152	ASN	10.6
1	A	148	ASN	10.5
1	A	98	THR	10.5
1	A	257	ALA	10.4
1	C	210	GLY	10.3
1	B	232	SER	10.2
1	B	143	VAL	10.1
1	B	148	ASN	10.1
1	A	260	LEU	10.0
1	C	48	ALA	10.0
1	C	64	ARG	10.0
1	C	177	SER	9.9
1	C	75	THR	9.8
1	B	253	PRO	9.6
1	B	82	ASP	9.6
1	A	155	GLY	9.5
1	B	176	CYS	9.3
1	C	47	SER	9.3
1	A	232	SER	9.2
1	C	122	SER	9.1
1	C	167	GLY	9.1
1	C	203	ALA	9.0
1	B	177	SER	9.0
1	B	216	ALA	8.9
1	A	175	ARG	8.9
1	A	180	SER	8.9
1	C	44	MET	8.8
1	A	203	ALA	8.7
1	A	88	SER	8.6
1	C	57	ASN	8.5
1	B	122	SER	8.5
1	B	76	ALA	8.5
1	C	148	ASN	8.5
1	B	83	SER	8.4
1	B	235	THR	8.4
1	C	43	SER	8.2
1	B	178	ASP	8.2
1	B	210	GLY	8.1
1	A	85	VAL	8.0
1	B	195	LYS	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	174	SER	8.0
1	B	206	ALA	7.9
1	B	151	SER	7.9
1	A	126	SER	7.8
1	A	102	GLY	7.8
1	C	41	GLY	7.8
1	C	175	ARG	7.8
1	C	95	THR	7.7
1	C	56	ARG	7.7
1	B	230	ASP	7.5
1	B	85	VAL	7.5
1	C	178	ASP	7.5
1	C	89	GLU	7.4
1	C	111	SER	7.4
1	B	207	THR	7.4
1	B	145	VAL	7.3
1	B	142	THR	7.3
1	C	182	ALA	7.3
1	C	50	GLY	7.3
1	C	154	ARG	7.3
1	A	146	SER	7.2
1	A	231	GLY	7.2
1	C	176	CYS	7.2
1	A	245	THR	7.2
1	C	102	GLY	7.1
1	C	238	ALA	7.1
1	B	160	GLN	7.0
1	A	195	LYS	7.0
1	C	194	LYS	7.0
1	B	238	ALA	6.9
1	B	77	GLU	6.9
1	B	126	SER	6.9
1	A	106	ASN	6.9
1	B	233	SER	6.8
1	C	88	SER	6.8
1	C	97	GLY	6.8
1	B	149	LYS	6.8
1	A	137	TYR	6.8
1	C	98	THR	6.7
1	A	105	ASP	6.7
1	C	105	ASP	6.7
1	C	179	THR	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	132	HIS	6.6
1	B	120	ILE	6.6
1	B	106	ASN	6.6
1	B	158	SER	6.6
1	A	125	SER	6.6
1	B	102	GLY	6.6
1	A	194	LYS	6.5
1	A	142	THR	6.5
1	C	65	GLY	6.5
1	A	123	CYS	6.5
1	A	214	ASN	6.4
1	A	207	THR	6.4
1	C	232	SER	6.4
1	C	213	VAL	6.4
1	B	152	ASN	6.4
1	A	160	GLN	6.4
1	C	173	ASN	6.4
1	C	45	ALA	6.3
1	B	193	GLY	6.3
1	C	67	ILE	6.3
1	A	124	PRO	6.3
1	B	179	THR	6.3
1	C	190	SER	6.3
1	B	121	PRO	6.2
1	B	90	LEU	6.2
1	C	40	ALA	6.2
1	A	77	GLU	6.2
1	C	168	LEU	6.2
1	B	200	LYS	6.2
1	C	90	LEU	6.2
1	C	82	ASP	6.0
1	C	125	SER	6.0
1	C	155	GLY	5.9
1	C	233	SER	5.9
1	A	230	ASP	5.9
1	B	136	GLN	5.9
1	B	159	GLY	5.9
1	B	138	ASP	5.8
1	C	99	TRP	5.8
1	A	154	ARG	5.8
1	B	154	ARG	5.8
1	C	70	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	151	SER	5.7
1	B	190	SER	5.7
1	A	181	THR	5.7
1	B	127	THR	5.7
1	C	191	GLU	5.7
1	A	244	ASP	5.6
1	A	122	SER	5.6
1	B	128	ALA	5.6
1	C	91	VAL	5.6
1	B	99	TRP	5.6
1	C	106	ASN	5.5
1	C	183	ILE	5.5
1	C	157	VAL	5.5
1	B	231	GLY	5.5
1	C	163	SER	5.5
1	C	255	ALA	5.5
1	A	159	GLY	5.5
1	A	156	TYR	5.5
1	A	229	LEU	5.5
1	A	89	GLU	5.5
1	B	181	THR	5.4
1	C	113	LEU	5.4
1	A	237	VAL	5.4
1	A	236	ALA	5.4
1	B	79	GLY	5.4
1	C	246	TYR	5.4
1	C	188	ASP	5.4
1	A	233	SER	5.4
1	C	42	ILE	5.4
1	C	204	ASP	5.3
1	A	127	THR	5.3
1	A	157	VAL	5.3
1	C	124	PRO	5.2
1	C	128	ALA	5.2
1	C	186	THR	5.2
1	A	196	TRP	5.2
1	C	52	MET	5.2
1	B	215	ILE	5.2
1	A	186	THR	5.2
1	B	247	THR	5.2
1	A	72	CYS	5.2
1	A	206	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	87	SER	5.2
1	A	217	THR	5.1
1	A	90	LEU	5.1
1	C	142	THR	5.1
1	C	160	GLN	5.1
1	C	249	GLN	5.1
1	C	243	TYR	5.1
1	A	253	PRO	5.1
1	C	189	VAL	5.0
1	C	237	VAL	5.0
1	C	253	PRO	5.0
1	C	251	ILE	5.0
1	A	255	ALA	5.0
1	C	143	VAL	5.0
1	B	191	GLU	5.0
1	C	73	GLU	5.0
1	C	118	THR	4.9
1	C	257	ALA	4.9
1	C	83	SER	4.9
1	B	189	VAL	4.9
1	C	151	SER	4.9
1	C	123	CYS	4.9
1	A	190	SER	4.9
1	B	87	SER	4.8
1	B	169	CYS	4.8
1	A	201	THR	4.8
1	C	220	VAL	4.8
1	C	217	THR	4.8
1	B	172	ASN	4.8
1	C	77	GLU	4.8
1	B	251	ILE	4.7
1	C	252	GLU	4.7
1	B	241	ARG	4.7
1	B	250	MET	4.7
1	B	125	SER	4.7
1	B	165	SER	4.7
1	C	108	SER	4.7
1	A	208	ALA	4.7
1	C	166	ALA	4.7
1	C	69	VAL	4.7
1	A	189	VAL	4.7
1	C	207	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	166	ALA	4.7
1	C	206	ALA	4.7
1	B	213	VAL	4.7
1	B	72	CYS	4.6
1	A	149	LYS	4.6
1	B	180	SER	4.6
1	A	141	ASP	4.6
1	C	196	TRP	4.6
1	B	229	LEU	4.6
1	B	103	VAL	4.6
1	A	73	GLU	4.6
1	C	55	ILE	4.6
1	C	137	TYR	4.6
1	B	194	LYS	4.6
1	A	128	ALA	4.6
1	B	163	SER	4.5
1	C	114	SER	4.5
1	C	228	LEU	4.5
1	A	204	ASP	4.5
1	A	83	SER	4.5
1	A	241	ARG	4.5
1	B	146	SER	4.5
1	B	166	ALA	4.5
1	B	220	VAL	4.5
1	C	116	ARG	4.5
1	C	53	VAL	4.4
1	B	243	TYR	4.4
1	B	70	LEU	4.4
1	C	218	ASP	4.4
1	A	95	THR	4.4
1	A	184	SER	4.4
1	A	144	PRO	4.4
1	A	66	ALA	4.4
1	C	219	LEU	4.4
1	C	242	ILE	4.4
1	A	202	SER	4.4
1	B	73	GLU	4.3
1	A	171	ILE	4.3
1	B	209	VAL	4.3
1	A	130	SER	4.3
1	A	198	PRO	4.3
1	A	165	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	61	SER	4.3
1	C	110	TYR	4.3
1	C	107	TRP	4.3
1	C	211	VAL	4.2
1	C	54	ARG	4.2
1	A	110	TYR	4.2
1	C	149	LYS	4.2
1	C	161	VAL	4.2
1	C	72	CYS	4.2
1	C	156	TYR	4.2
1	C	85	VAL	4.2
1	C	152	ASN	4.2
1	A	222	ALA	4.1
1	B	256	SER	4.1
1	B	124	PRO	4.1
1	B	71	HIS	4.1
1	C	147	VAL	4.1
1	B	252	GLU	4.1
1	C	84	ILE	4.1
1	A	119	TYR	4.1
1	B	114	SER	4.0
1	C	230	ASP	4.0
1	B	139	MET	4.0
1	A	239	ALA	4.0
1	B	104	ALA	4.0
1	A	212	ASP	4.0
1	B	184	SER	4.0
1	B	204	ASP	4.0
1	A	234	SER	4.0
1	A	134	GLY	4.0
1	A	169	CYS	4.0
1	B	259	ASN	3.9
1	B	260	LEU	3.9
1	B	74	LEU	3.9
1	A	68	THR	3.9
1	B	245	THR	3.9
1	A	188	ASP	3.9
1	A	113	LEU	3.9
1	A	224	LEU	3.9
1	B	68	THR	3.9
1	C	185	THR	3.9
1	C	254	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	193	GLY	3.9
1	A	226	ILE	3.9
1	B	218	ASP	3.9
1	A	223	ARG	3.8
1	C	58	PRO	3.8
1	C	214	ASN	3.8
1	B	202	SER	3.8
1	B	212	ASP	3.8
1	C	244	ASP	3.8
1	A	209	VAL	3.8
1	C	133	MET	3.8
1	C	170	PHE	3.8
1	B	88	SER	3.8
1	C	146	SER	3.8
1	C	66	ALA	3.8
1	A	69	VAL	3.8
1	A	211	VAL	3.8
1	B	89	GLU	3.8
1	B	81	THR	3.8
1	B	129	GLY	3.8
1	B	203	ALA	3.8
1	B	86	VAL	3.8
1	A	131	ILE	3.8
1	C	49	GLN	3.8
1	A	163	SER	3.8
1	C	120	ILE	3.8
1	B	113	LEU	3.8
1	C	260	LEU	3.8
1	C	169	CYS	3.8
1	A	249	GLN	3.7
1	C	138	ASP	3.7
1	B	150	LEU	3.7
1	A	94	TYR	3.7
1	B	205	TYR	3.7
1	C	101	ARG	3.7
1	A	246	TYR	3.7
1	A	136	GLN	3.7
1	A	219	LEU	3.7
1	C	240	GLY	3.7
1	A	108	SER	3.7
1	A	147	VAL	3.7
1	C	68	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	78	ILE	3.7
1	C	201	THR	3.6
1	C	74	LEU	3.6
1	B	107	TRP	3.6
1	A	104	ALA	3.6
1	A	111	SER	3.6
1	B	234	SER	3.6
1	B	168	LEU	3.6
1	C	135	PHE	3.6
1	B	80	VAL	3.6
1	A	121	PRO	3.6
1	A	252	GLU	3.6
1	C	162	TRP	3.5
1	B	75	THR	3.5
1	B	219	LEU	3.5
1	C	159	GLY	3.5
1	B	95	THR	3.5
1	C	139	MET	3.5
1	A	107	TRP	3.5
1	C	245	THR	3.4
1	A	158	SER	3.4
1	A	251	ILE	3.4
1	C	94	TYR	3.4
1	A	145	VAL	3.4
1	A	129	GLY	3.4
1	A	259	ASN	3.4
1	A	221	PRO	3.4
1	B	171	ILE	3.4
1	A	82	ASP	3.4
1	B	258	LEU	3.4
1	B	112	TRP	3.4
1	B	228	LEU	3.4
1	C	60	VAL	3.4
1	C	104	ALA	3.4
1	A	120	ILE	3.4
1	C	259	ASN	3.3
1	B	157	VAL	3.3
1	A	193	GLY	3.3
1	C	141	ASP	3.3
1	C	199	TYR	3.3
1	C	81	THR	3.3
1	B	153	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	109	LYS	3.3
1	A	84	ILE	3.3
1	A	197	TYR	3.3
1	B	110	TYR	3.3
1	B	100	LEU	3.3
1	B	67	ILE	3.2
1	C	236	ALA	3.2
1	C	109	LYS	3.2
1	C	158	SER	3.2
1	C	198	PRO	3.2
1	C	86	VAL	3.2
1	B	108	SER	3.2
1	A	116	ARG	3.2
1	B	66	ALA	3.2
1	B	164	GLY	3.2
1	C	239	ALA	3.2
1	C	215	ILE	3.1
1	B	155	GLY	3.1
1	C	119	TYR	3.1
1	A	70	LEU	3.1
1	C	145	VAL	3.1
1	C	140	ALA	3.1
1	B	185	THR	3.1
1	C	165	SER	3.1
1	B	192	LEU	3.1
1	C	71	HIS	3.1
1	A	81	THR	3.1
1	B	84	ILE	3.1
1	A	99	TRP	3.0
1	B	183	ILE	3.0
1	A	101	ARG	3.0
1	C	231	GLY	3.0
1	A	115	VAL	3.0
1	B	186	THR	3.0
1	A	162	TRP	3.0
1	A	67	ILE	3.0
1	A	258	LEU	3.0
1	B	140	ALA	3.0
1	C	212	ASP	3.0
1	A	138	ASP	3.0
1	B	249	GLN	3.0
1	A	254	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	114	SER	3.0
1	A	227	ALA	3.0
1	C	256	SER	3.0
1	A	117	TYR	3.0
1	B	188	ASP	3.0
1	C	46	PRO	2.9
1	A	71	HIS	2.9
1	A	91	VAL	2.9
1	B	239	ALA	2.9
1	A	86	VAL	2.9
1	B	211	VAL	2.9
1	A	74	LEU	2.9
1	A	238	ALA	2.9
1	B	222	ALA	2.8
1	B	98	THR	2.8
1	A	168	LEU	2.8
1	B	240	GLY	2.8
1	A	243	TYR	2.8
1	C	117	TYR	2.8
1	B	170	PHE	2.8
1	B	187	LEU	2.8
1	B	133	MET	2.7
1	C	100	LEU	2.7
1	A	191	GLU	2.7
1	B	134	GLY	2.7
1	B	116	ARG	2.7
1	A	164	GLY	2.7
1	A	96	VAL	2.7
1	C	216	ALA	2.7
1	A	100	LEU	2.7
1	B	248	ILE	2.7
1	C	222	ALA	2.7
1	C	78	ILE	2.6
1	B	118	THR	2.6
1	B	254	THR	2.6
1	B	147	VAL	2.6
1	B	237	VAL	2.6
1	A	228	LEU	2.6
1	B	119	TYR	2.6
1	A	218	ASP	2.6
1	B	167	GLY	2.6
1	A	213	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	255	ALA	2.6
1	C	121	PRO	2.6
1	B	227	ALA	2.6
1	A	220	VAL	2.5
1	A	182	ALA	2.5
1	C	258	LEU	2.5
1	A	161	VAL	2.5
1	B	236	ALA	2.5
1	C	150	LEU	2.5
1	C	103	VAL	2.5
1	B	201	THR	2.5
1	C	181	THR	2.5
1	B	141	ASP	2.4
1	C	171	ILE	2.4
1	A	170	PHE	2.4
1	A	150	LEU	2.4
1	A	179	THR	2.4
1	B	225	VAL	2.4
1	C	79	GLY	2.4
1	B	198	PRO	2.4
1	A	205	TYR	2.3
1	C	76	ALA	2.3
1	C	250	MET	2.3
1	B	132	HIS	2.3
1	B	94	TYR	2.3
1	B	111	SER	2.3
1	C	112	TRP	2.3
1	B	135	PHE	2.3
1	A	109	LYS	2.3
1	A	200	LYS	2.3
1	A	93	PRO	2.3
1	C	229	LEU	2.3
1	A	256	SER	2.3
1	C	223	ARG	2.3
1	B	244	ASP	2.3
1	C	205	TYR	2.2
1	C	209	VAL	2.2
1	B	242	ILE	2.2
1	B	224	LEU	2.2
1	C	192	LEU	2.2
1	C	51	ALA	2.2
1	C	129	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	196	TRP	2.2
1	C	172	ASN	2.2
1	B	93	PRO	2.2
1	B	182	ALA	2.2
1	B	123	CYS	2.2
1	C	200	LYS	2.1
1	A	250	MET	2.1
1	C	227	ALA	2.1
1	C	130	SER	2.1
1	C	197	TYR	2.1
1	B	161	VAL	2.1
1	A	183	ILE	2.1
1	A	139	MET	2.1
1	A	199	TYR	2.1
1	B	137	TYR	2.1
1	A	242	ILE	2.0
1	B	223	ARG	2.0
1	C	241	ARG	2.0
1	A	75	THR	2.0
1	C	93	PRO	2.0
1	C	59	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	CA	A	304	1/1	0.62	0.36	2,2,2,2	0
2	CA	A	300	1/1	0.78	0.29	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	303	1/1	0.84	0.25	10,10,10,10	0
2	CA	C	302	1/1	0.91	0.30	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.