



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 09:11 AM EDT

PDB ID : 2C6S / pdb_00002c6s
Title : human adenovirus penton base 2 12 chimera
Authors : Zubieta, C.; Blanchoin, L.; Cusack, S.
Deposited on : 2005-11-11
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

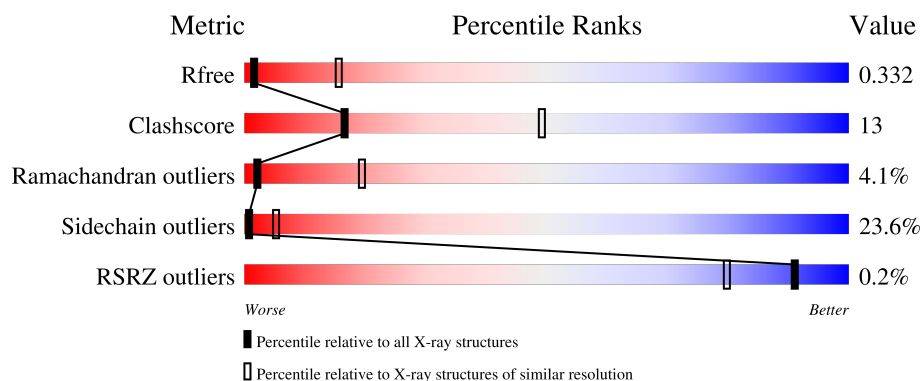
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	523	37% 32% 14% • 15%
1	B	523	35% 33% 13% • 15%
1	C	523	37% 32% 13% • 15%
1	D	523	39% 31% 11% • 15%
1	E	523	35% 33% 15% • 15%

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Mol	Chain	Length	Quality of chain
1	F	523	
1	G	523	
1	H	523	
1	I	523	
1	J	523	
1	K	523	
1	L	523	
1	M	523	
1	N	523	
1	O	523	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53010 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 ADENOVIRUS 2,12 PENTON BASE CHIMERA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	B	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	C	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	D	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	E	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	F	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	G	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	H	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	I	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	J	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	K	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	L	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	M	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	N	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	O	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			

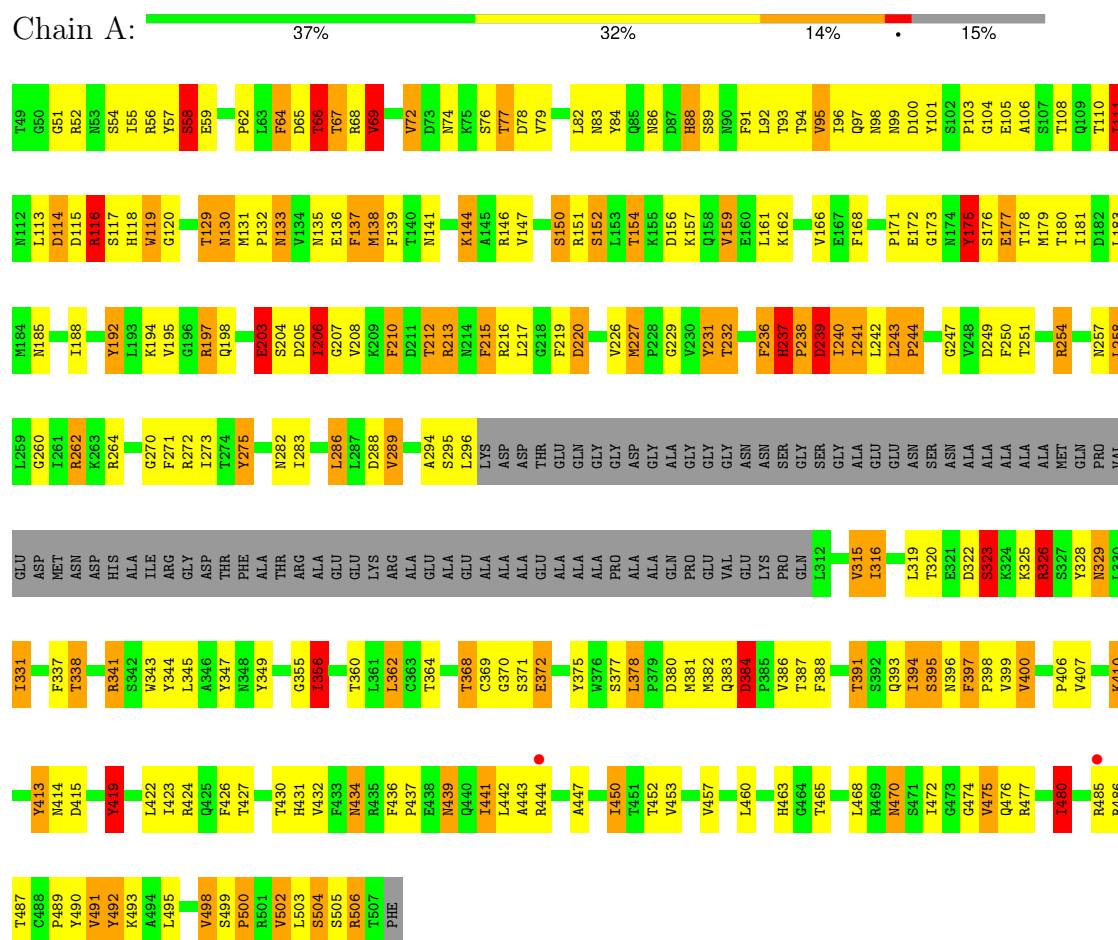
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	LEU	LYS	conflict	UNP P03276
B	312	LEU	LYS	conflict	UNP P03276
C	312	LEU	LYS	conflict	UNP P03276
D	312	LEU	LYS	conflict	UNP P03276
E	312	LEU	LYS	conflict	UNP P03276
F	312	LEU	LYS	conflict	UNP P03276
G	312	LEU	LYS	conflict	UNP P03276
H	312	LEU	LYS	conflict	UNP P03276
I	312	LEU	LYS	conflict	UNP P03276
J	312	LEU	LYS	conflict	UNP P03276
K	312	LEU	LYS	conflict	UNP P03276
L	312	LEU	LYS	conflict	UNP P03276
M	312	LEU	LYS	conflict	UNP P03276
N	312	LEU	LYS	conflict	UNP P03276
O	312	LEU	LYS	conflict	UNP P03276

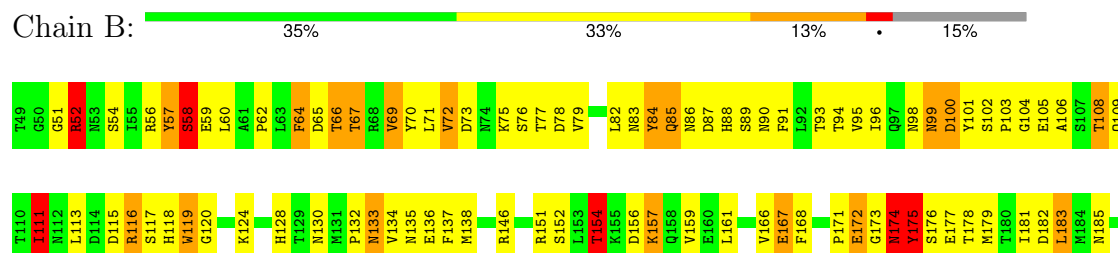
3 Residue-property plots

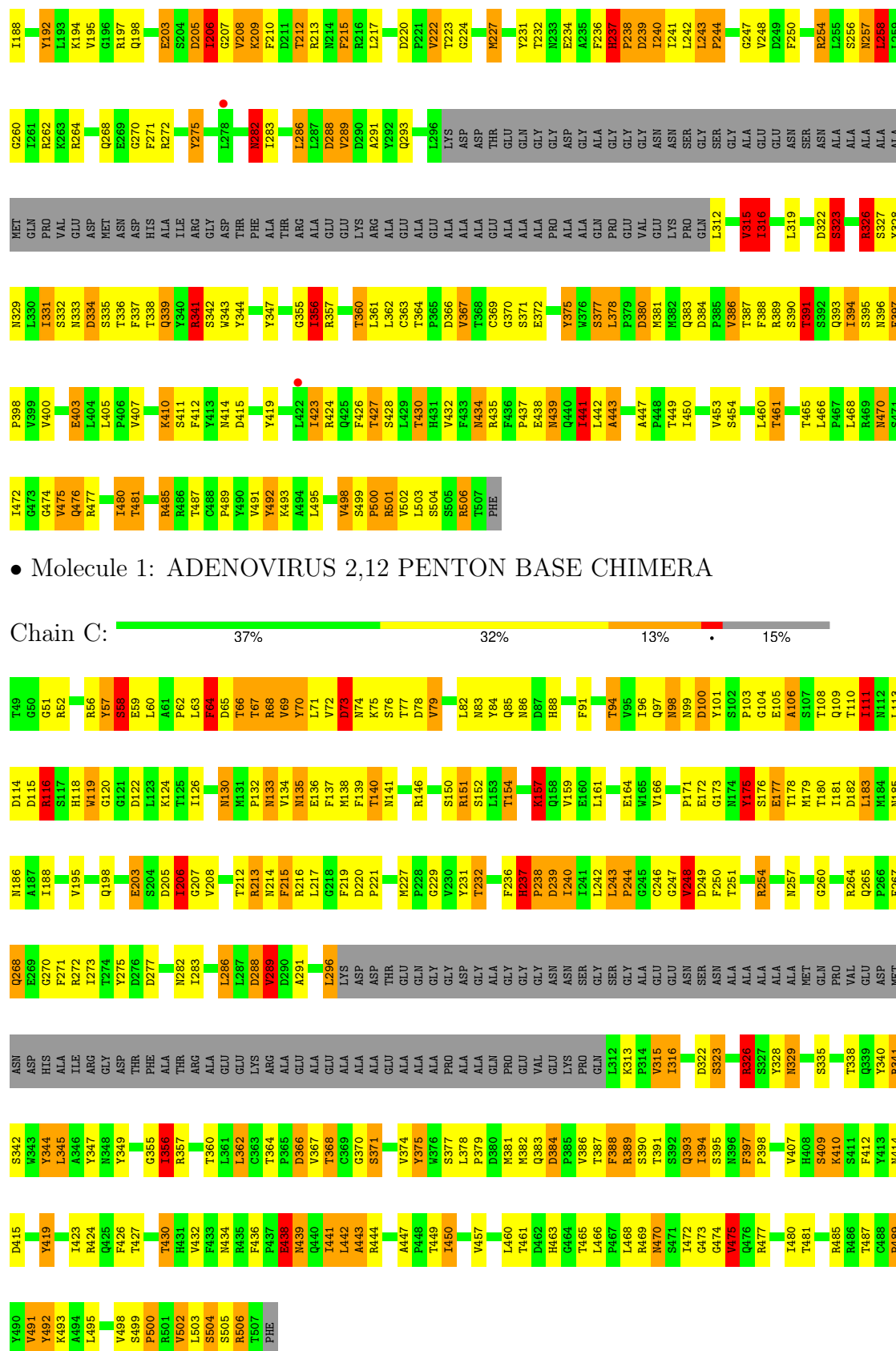
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ADENOVIRUS 2,12 PENTON BASE CHIMERA

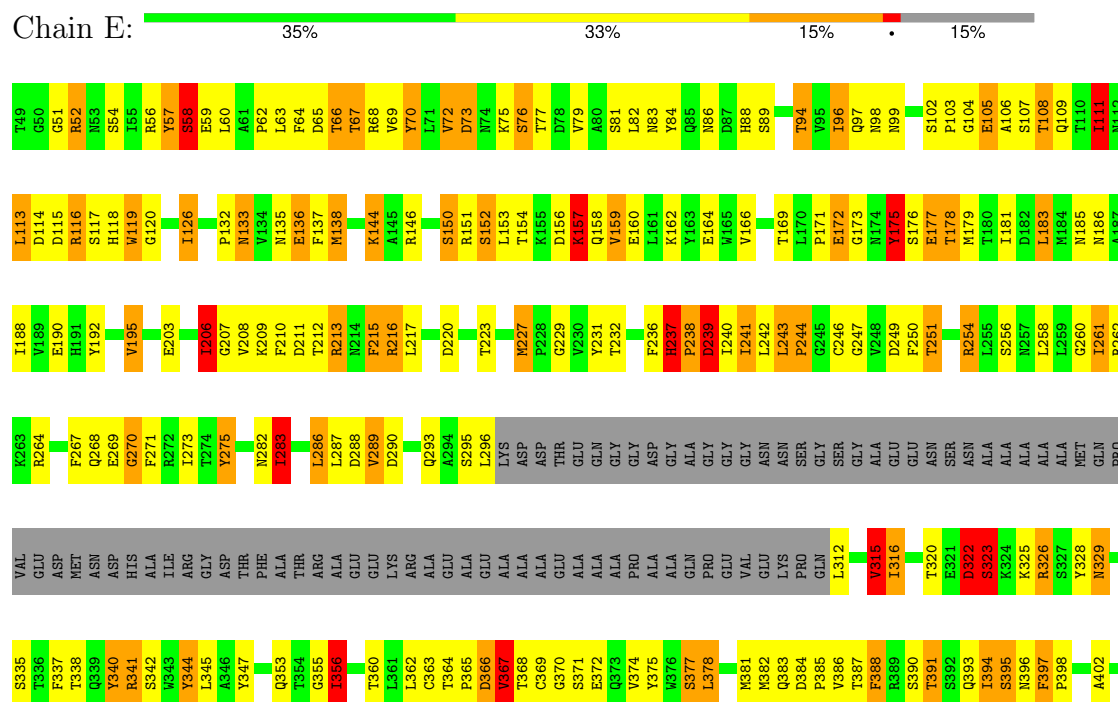
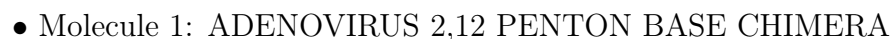


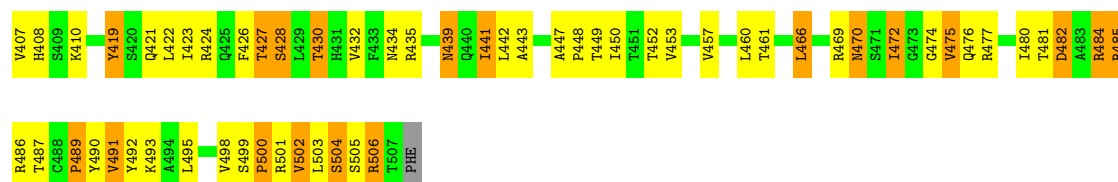
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA



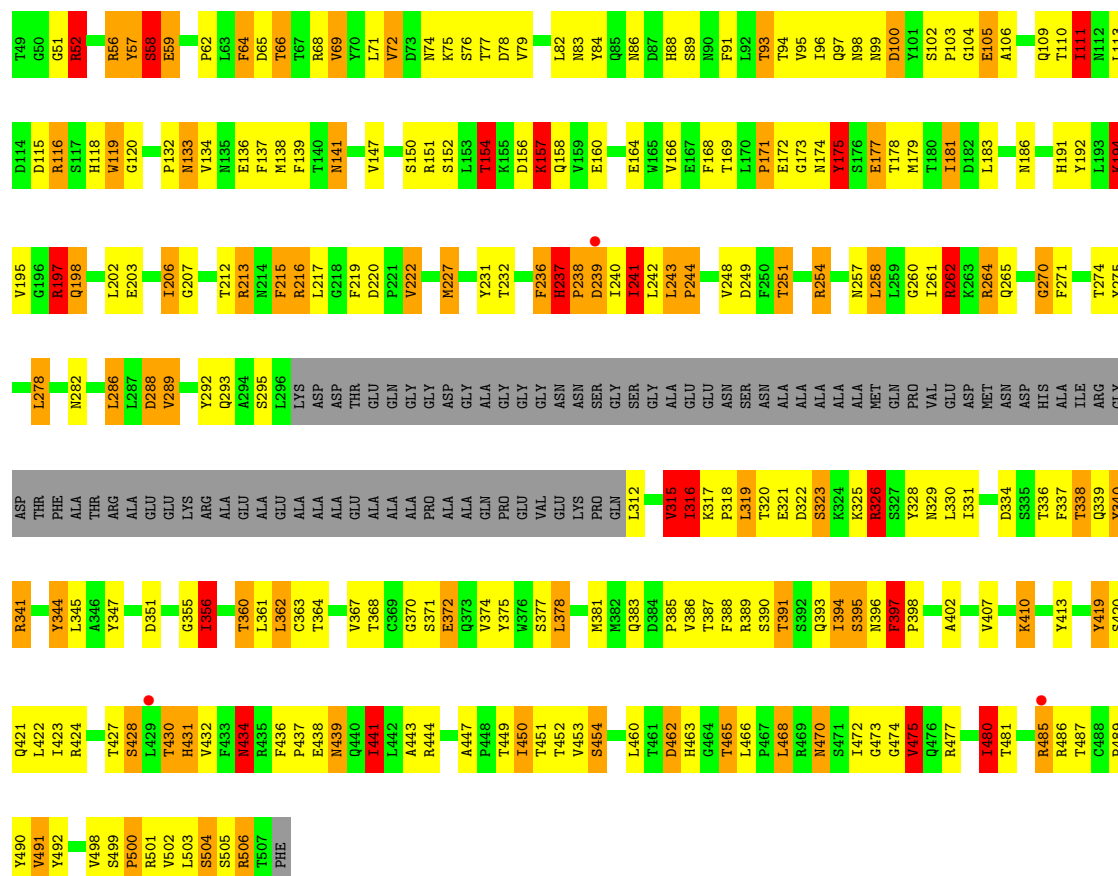


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

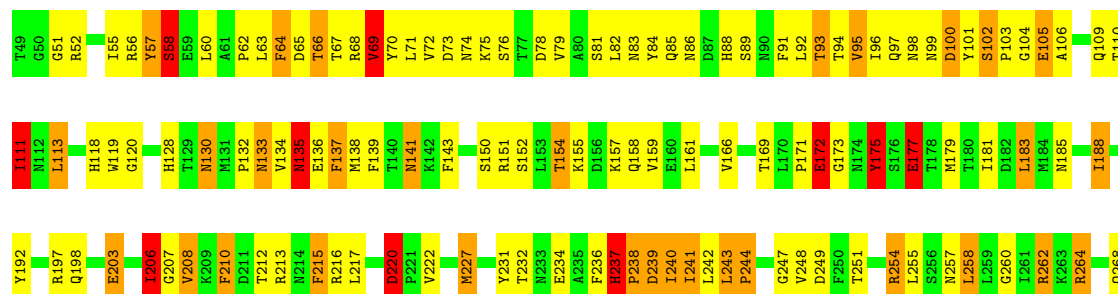
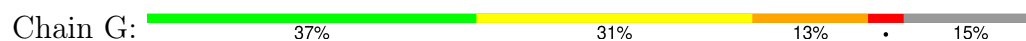


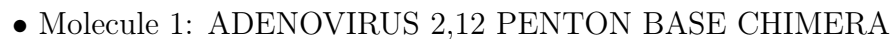


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

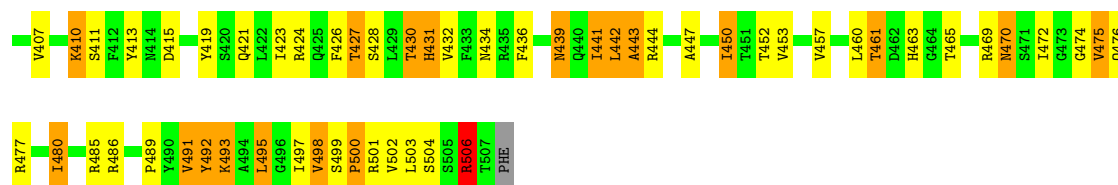


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA



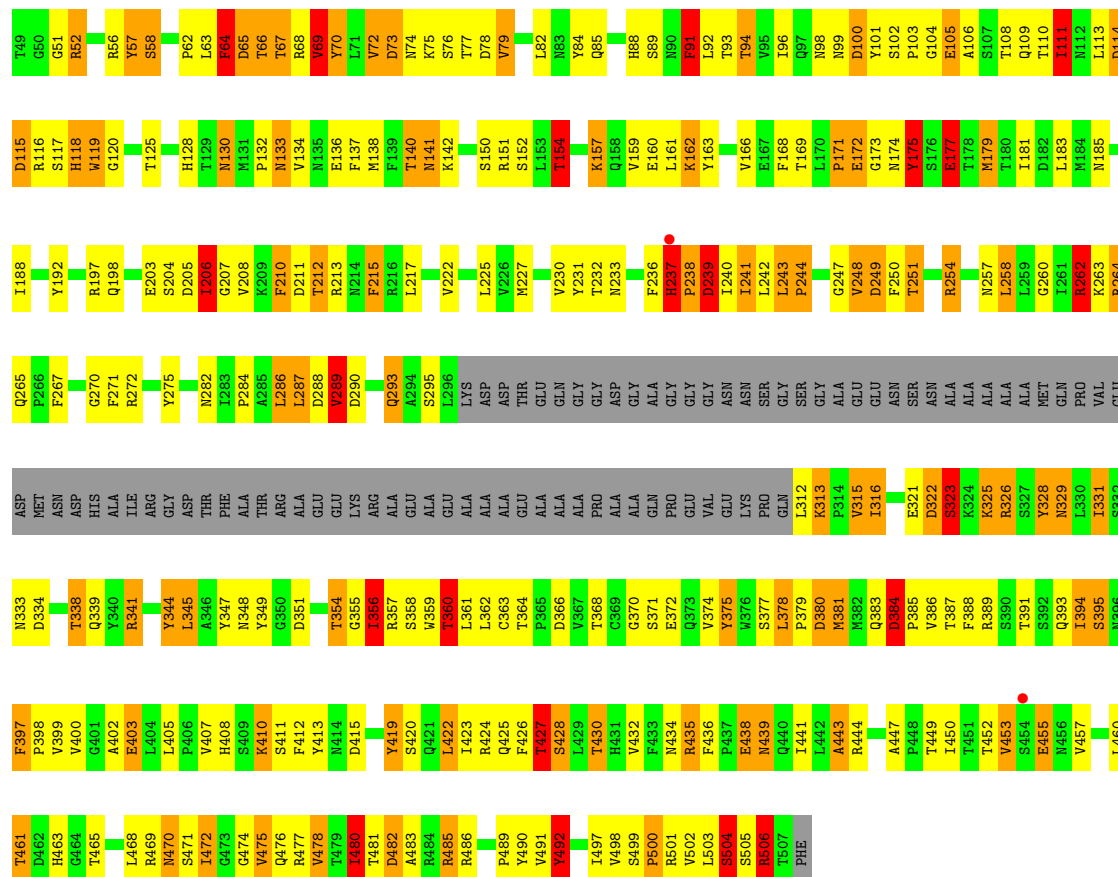


A	Y328	ALA	R254	L183	D114	T49	
	N329	ALA	L255	M184	D115	G50	
	L330	ALA	S256	N185	D116	G51	
	I331	GLN	N257	M186	R117	R52	
	D	D334	PRO	L258	A187	S117	N53
		S335	VAL	G260	I188	H118	S54
		T336	GLU	T261		I119	I95
	F337	GLU	R262	Y192	G120	R56	
	T338	MET	K263	L193	K124	S58	
	E	Y341	ASN	R264	K194	T125	E59
R341		ASP	Q268	R197	L126	P62	
S342		HIS		L127	L63	P64	
W343		ALA		H128	D65	D66	
Y344		ILE	G270	Q198	T129	T67	
L345		ARG	F271	V201	M130	V69	
L346		GLY	R272	S204	K131	L71	
Y347		ASP	T273	D205	P132	V72	
D351		THR	T274	T206	M133	D73	
F		G355	ALA	Y275	G207	V134	K75
	L356	ALA	N282	V208	N135	T77	
		THR	L286	K209	E136	D78	
		ARG		F137	L70	W79	
	ALA	D210		K144	L82		
	T360	GLU	L287	D211	R151	N83	
	L361	GLU	R288	D212	S152	Y84	
	L362	LVS	V289	T212	L153	Q85	
	G	Y367	ARG	D290	N214	T154	N86
		T368	GLU	A291	D215	K155	D87
G369		ALA	S295	R216	K157	H88	
H	G370	GLU	L296	L217	E160	N90	
	S371	ALA	LVS	D220	S150	L92	
	Y374	ALA	ASP	V226	R151	T93	
	Y375	GLU	THR		R152	T94	
	K376	ALA	GLU		L153	V166	
	F377	ALA	GLN	M227	E167	V95	
	L378	ALA	GLY	V231	F168	I96	
	F379	PRO	GLY	T232	T169	Q87	
	I	M382	ALA	ASP	N233	L170	N98
			ALA	GLY	E234	P171	N99
GLN			A235	G172	D100		
Q383		PRO	GLY	F236	E172	Y101	
D384		GLU	GLY	R237	G173	S102	
L386		VAL	GLY	P238	N174	P103	
T387		GLU	ASN	D239	K175	L104	
F388		LVS	ASN	T240	S176	G104	
R389		PRO	SER	T241	E177	E106	
S390		GLN	SER	L242	M178	A106	
J	T391	L312	SER	L243	G179	Q109	
	S392	L315	ALA	P244	N175		T181
	Q393	I316	ALA	G247	S176		L192
	L394	S395	ALA	V248	T178	R193	
	N396	D322	ASN	D249	L178	Q109	
	F397	S323	SER	F250	M179		T180
	T398	ASN	ASN	T251	T180		L181
	Y403	R326	ALA	H252	K192	R193	
	K	L356	ALA	LVS	D220	S150	L82
			ALA	ASP	R151	R83	
ALA			ASP	S152	Y84		
Y374		GLU	THR	V226	L153	Q85	
K376		ALA	GLU	M227	T154	N86	
F377		ALA	GLN	V231	K155	D87	
L378		ALA	GLY	T232	K157	H88	
F379		PRO	GLY	N233	Q158	N90	
L		M382	ALA	ASP	V159	F91	
			ALA	GLY	E160	L92	
	GLN		A235	T93			
	Q383	PRO	GLY	F236	V166	T94	
	D384	GLU	GLY	R237	E167	V95	
	L386	VAL	GLY	P238	F168	I96	
	T387	GLU	ASN	D239	T169	Q87	
	F388	LVS	ASN	T240	L170	N98	
	R389	PRO	SER	T241	P171	N99	
	S390	L312	SER	L242	E172	D100	
M	S392	L315	ALA	P244	G173	Y101	
	Q393	I316	ALA	G247	N174	S102	
	L394	S395	ALA	V248	K175	L104	
	N396	D322	ASN	D249	S176	G104	
	F397	S323	SER	F250	E177	E106	
	T398	ASN	ASN	T251	M179	A106	
	Y403	R326	ALA	H252	T180	T181	
	N	L356	ALA	LVS	D220	S150	L82
			ALA	ASP	R151	R83	
			ALA	ASP	S152	Y84	
Y374		GLU	THR	V226	L153	Q85	
K376		ALA	GLU</				



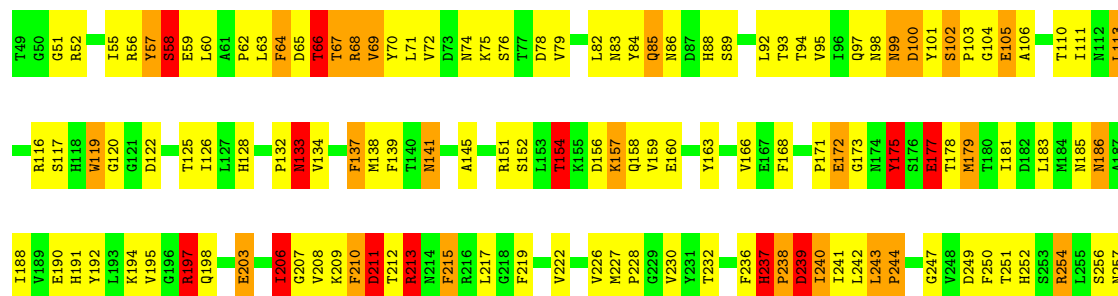
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

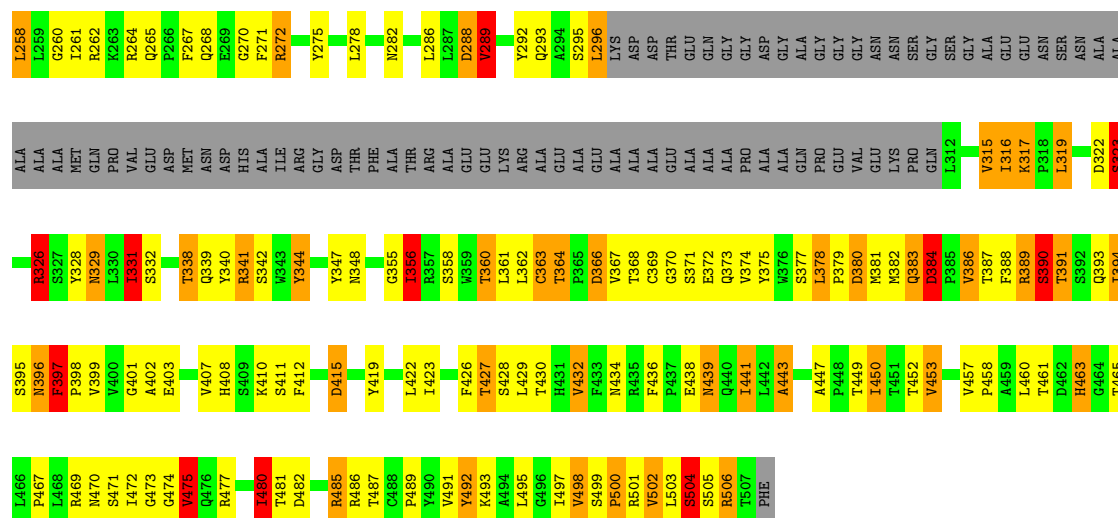
Chain K: 32% 33% 16% 15%



• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

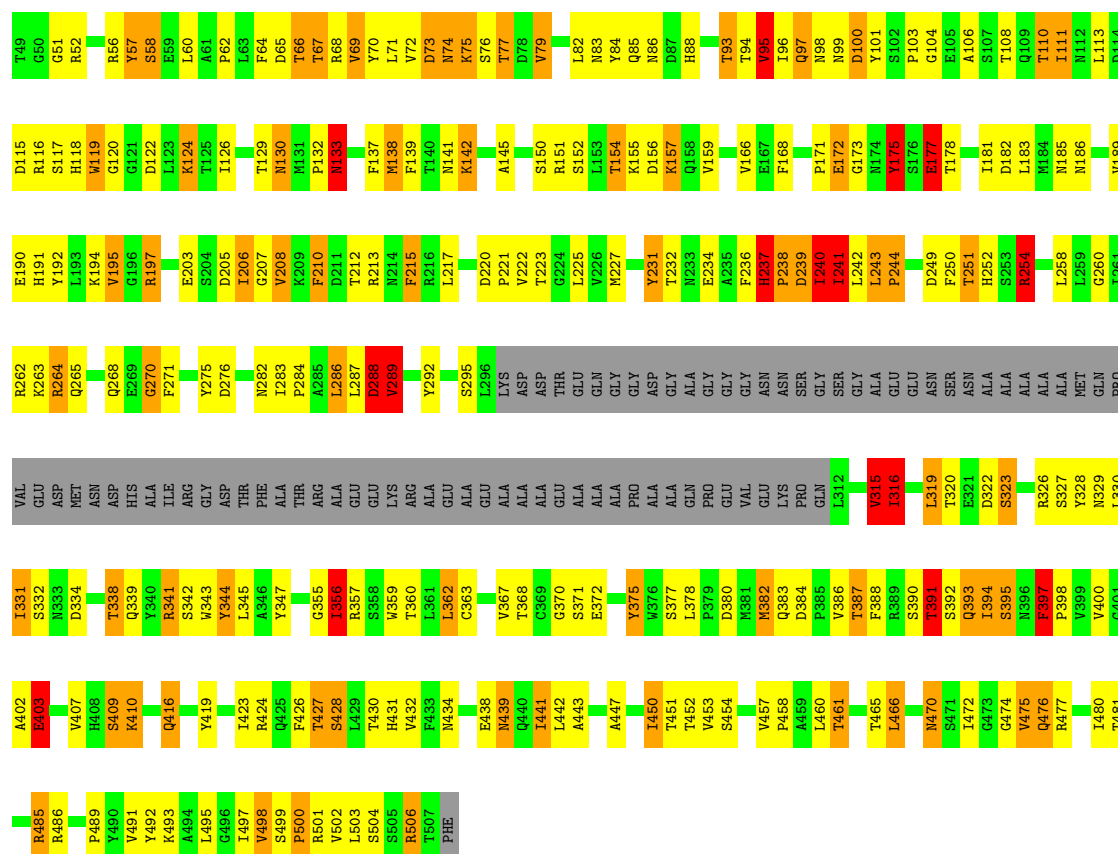
Chain L: 33% 35% 12% 15%





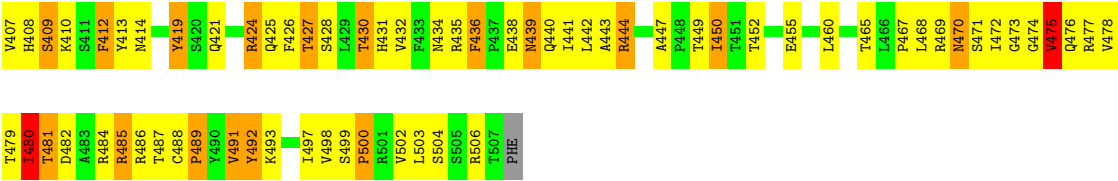
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain M: 36% 33% 13% 15%



• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain N: 33% 35% 13% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	266.50Å 292.90Å 307.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.60 15.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.60) 88.0 (15.00-3.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.275 , 0.340 0.277 , 0.332	Depositor DCC
R_{free} test set	3041 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	131.0	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	53010	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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	1.12	15/3617 (0.4%)	1.29	18/4926 (0.4%)
1	B	1.28	25/3617 (0.7%)	1.36	25/4926 (0.5%)
1	C	1.25	19/3617 (0.5%)	1.32	20/4926 (0.4%)
1	D	1.14	11/3617 (0.3%)	1.33	19/4926 (0.4%)
1	E	1.18	21/3617 (0.6%)	1.32	17/4926 (0.3%)
1	F	1.25	23/3617 (0.6%)	1.34	23/4926 (0.5%)
1	G	1.28	21/3617 (0.6%)	1.33	25/4926 (0.5%)
1	H	1.15	12/3617 (0.3%)	1.30	15/4926 (0.3%)
1	I	1.10	7/3617 (0.2%)	1.32	19/4926 (0.4%)
1	J	1.16	22/3617 (0.6%)	1.31	21/4926 (0.4%)
1	K	1.23	23/3617 (0.6%)	1.34	18/4926 (0.4%)
1	L	1.14	17/3617 (0.5%)	1.33	21/4926 (0.4%)
1	M	1.30	31/3617 (0.9%)	1.37	23/4926 (0.5%)
1	N	1.18	16/3617 (0.4%)	1.34	27/4926 (0.5%)
1	O	1.33	34/3617 (0.9%)	1.38	25/4926 (0.5%)
All	All	1.21	297/54255 (0.5%)	1.33	316/73890 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	109
1	B	0	105
1	C	0	111
1	D	0	107
1	E	0	103
1	F	0	108
1	G	0	113
1	H	0	114
1	I	0	115
1	J	0	112

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	119
1	L	0	115
1	M	0	105
1	N	0	116
1	O	0	115
All	All	0	1667

The worst 5 of 297 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	220	ASP	CG-OD2	22.53	1.68	1.25
1	C	157	LYS	CE-NZ	19.25	2.07	1.49
1	F	326	ARG	CZ-NH1	17.57	1.57	1.32
1	O	372	GLU	CD-OE1	16.91	1.57	1.25
1	F	194	LYS	CE-NZ	16.47	1.98	1.49

The worst 5 of 316 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	ARG	NE-CZ-NH2	-13.33	107.20	119.20
1	C	157	LYS	CG-CD-CE	-12.19	83.26	111.30
1	F	227	MET	CA-C-N	-10.59	106.61	119.84
1	F	227	MET	C-N-CA	-10.59	106.61	119.84
1	I	227	MET	CA-C-N	-10.52	106.69	119.84

There are no chirality outliers.

5 of 1667 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	ARG	Mainchain
1	A	56	ARG	Mainchain,Sidechain
1	A	57	TYR	Sidechain
1	A	58	SER	Mainchain
1	A	62	PRO	Mainchain

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	3534	0	3463	85	0
1	B	3534	0	3463	107	0
1	C	3534	0	3463	101	0
1	D	3534	0	3463	82	0
1	E	3534	0	3463	106	0
1	F	3534	0	3463	95	0
1	G	3534	0	3463	91	0
1	H	3534	0	3463	86	0
1	I	3534	0	3463	99	0
1	J	3534	0	3463	109	0
1	K	3534	0	3463	109	0
1	L	3534	0	3463	106	0
1	M	3534	0	3463	93	0
1	N	3534	0	3463	100	0
1	O	3534	0	3463	92	0
All	All	53010	0	51945	1350	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.

The worst 5 of 1350 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:J:124:LYS:CG	1:J:124:LYS:CD	1.78	1.62
1:K:422:LEU:CG	1:K:422:LEU:CD2	1.76	1.62
1:E:157:LYS:CE	1:E:157:LYS:CD	1.81	1.59
1:O:162:LYS:CE	1:O:162:LYS:CD	1.77	1.59
1:B:167:GLU:CD	1:B:167:GLU:CG	1.76	1.58

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	440/523 (84%)	357 (81%)	65 (15%)	18 (4%)	2	19
1	B	440/523 (84%)	360 (82%)	62 (14%)	18 (4%)	2	19
1	C	440/523 (84%)	357 (81%)	65 (15%)	18 (4%)	2	19
1	D	440/523 (84%)	360 (82%)	62 (14%)	18 (4%)	2	19
1	E	440/523 (84%)	358 (81%)	63 (14%)	19 (4%)	2	18
1	F	440/523 (84%)	359 (82%)	62 (14%)	19 (4%)	2	18
1	G	440/523 (84%)	359 (82%)	63 (14%)	18 (4%)	2	19
1	H	440/523 (84%)	359 (82%)	63 (14%)	18 (4%)	2	19
1	I	440/523 (84%)	360 (82%)	62 (14%)	18 (4%)	2	19
1	J	440/523 (84%)	358 (81%)	64 (14%)	18 (4%)	2	19
1	K	440/523 (84%)	356 (81%)	65 (15%)	19 (4%)	2	18
1	L	440/523 (84%)	359 (82%)	63 (14%)	18 (4%)	2	19
1	M	440/523 (84%)	358 (81%)	64 (14%)	18 (4%)	2	19
1	N	440/523 (84%)	361 (82%)	61 (14%)	18 (4%)	2	19
1	O	440/523 (84%)	361 (82%)	61 (14%)	18 (4%)	2	19
All	All	6600/7845 (84%)	5382 (82%)	945 (14%)	273 (4%)	2	19

5 of 273 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	172	GLU
1	A	237	HIS
1	A	286	LEU
1	A	323	SER

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	400/451 (89%)	304 (76%)	96 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	400/451 (89%)	318 (80%)	82 (20%)	1	8
1	C	400/451 (89%)	312 (78%)	88 (22%)	1	6
1	D	400/451 (89%)	307 (77%)	93 (23%)	1	5
1	E	400/451 (89%)	310 (78%)	90 (22%)	1	6
1	F	400/451 (89%)	311 (78%)	89 (22%)	1	6
1	G	400/451 (89%)	307 (77%)	93 (23%)	1	5
1	H	400/451 (89%)	301 (75%)	99 (25%)	1	4
1	I	400/451 (89%)	312 (78%)	88 (22%)	1	6
1	J	400/451 (89%)	307 (77%)	93 (23%)	1	5
1	K	400/451 (89%)	287 (72%)	113 (28%)	0	3
1	L	400/451 (89%)	298 (74%)	102 (26%)	0	4
1	M	400/451 (89%)	303 (76%)	97 (24%)	1	5
1	N	400/451 (89%)	297 (74%)	103 (26%)	0	4
1	O	400/451 (89%)	312 (78%)	88 (22%)	1	6
All	All	6000/6765 (89%)	4586 (76%)	1414 (24%)	1	5

5 of 1414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	108	THR
1	M	155	LYS
1	K	233	ASN
1	K	105	GLU
1	L	110	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 174 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	97	GLN
1	M	112	ASN
1	K	191	HIS
1	L	133	ASN
1	N	74	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	444/523 (84%)	-0.26	2 (0%) 87 66	96, 131, 195, 200	0
1	B	444/523 (84%)	-0.25	2 (0%) 87 66	96, 131, 195, 200	0
1	C	444/523 (84%)	-0.25	0 100 100	95, 131, 196, 200	0
1	D	444/523 (84%)	-0.24	0 100 100	96, 131, 195, 200	0
1	E	444/523 (84%)	-0.23	0 100 100	96, 131, 195, 200	0
1	F	444/523 (84%)	-0.21	3 (0%) 84 61	94, 131, 196, 200	0
1	G	444/523 (84%)	-0.22	0 100 100	94, 132, 195, 200	0
1	H	444/523 (84%)	-0.18	0 100 100	95, 131, 195, 200	0
1	I	444/523 (84%)	-0.24	1 (0%) 91 80	96, 131, 195, 200	0
1	J	444/523 (84%)	-0.17	0 100 100	95, 131, 196, 200	0
1	K	444/523 (84%)	-0.16	2 (0%) 87 66	96, 131, 196, 200	0
1	L	444/523 (84%)	-0.22	0 100 100	95, 131, 196, 200	0
1	M	444/523 (84%)	-0.23	0 100 100	95, 132, 196, 200	0
1	N	444/523 (84%)	-0.17	4 (0%) 81 56	95, 131, 196, 200	0
1	O	444/523 (84%)	-0.12	2 (0%) 87 66	94, 131, 195, 200	0
All	All	6660/7845 (84%)	-0.21	16 (0%) 91 80	94, 131, 196, 200	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	239	ASP	4.1
1	N	444	ARG	3.1
1	F	239	ASP	2.9
1	O	239	ASP	2.8
1	K	237	HIS	2.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.