



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:16 PM UTC

PDB ID : 3GV2 / pdb_00003gv2
Title : X-ray Structure of Hexameric HIV-1 CA
Authors : Kelly, B.N.
Deposited on : 2009-03-30
Resolution : 7.00 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

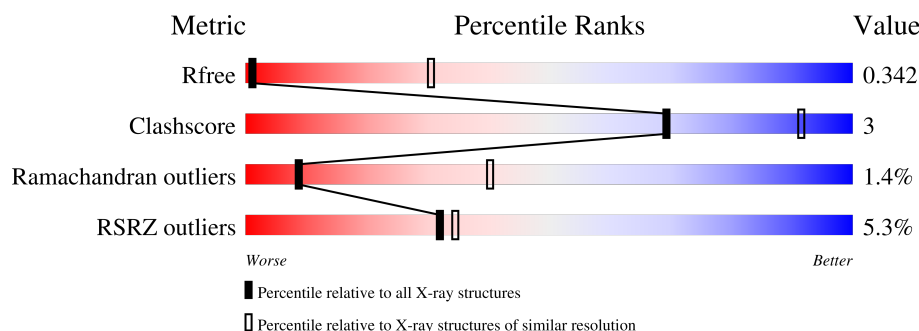
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	1167 (10.00-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	342	4% 58% 36%
1	B	342	2% 60% 36%
1	C	342	5% 59% 36%
1	D	342	4% 58% 5% 36%
1	E	342	2% 59% 36%
1	F	342	3% 59% 36%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5256 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 Capsid protein p24,Carbon dioxide-concentrating mechanism protein CcmK homolog 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	0	0	0
			876	438	219	219			
1	B	219	Total	C	N	O	0	0	0
			876	438	219	219			
1	C	219	Total	C	N	O	0	0	0
			876	438	219	219			
1	D	219	Total	C	N	O	0	0	0
			876	438	219	219			
1	E	219	Total	C	N	O	0	0	0
			876	438	219	219			
1	F	219	Total	C	N	O	0	0	0
			876	438	219	219			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ALA	TRP	engineered mutation	UNP P12493
A	185	ALA	MET	engineered mutation	UNP P12493
A	220	GLY	-	linker	UNP P12493
A	221	VAL	-	linker	UNP P12493
A	222	GLY	-	linker	UNP P12493
A	223	GLY	-	linker	UNP P12493
A	224	THR	-	linker	UNP P12493
A	225	ARG	-	linker	UNP P12493
A	226	PRO	-	linker	UNP P12493
A	227	GLU	-	linker	UNP P12493
A	228	LEU	-	linker	UNP P12493
A	332	TYR	GLU	conflict	UNP P73407
A	338	GLU	ASN	conflict	UNP P73407
A	339	VAL	-	expression tag	UNP P73407
A	340	LEU	-	expression tag	UNP P73407
A	341	PHE	-	expression tag	UNP P73407

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Chain	Residue	Modelled	Actual	Comment	Reference
A	342	GLN	-	expression tag	UNP P73407
B	184	ALA	TRP	engineered mutation	UNP P12493
B	185	ALA	MET	engineered mutation	UNP P12493
B	220	GLY	-	linker	UNP P12493
B	221	VAL	-	linker	UNP P12493
B	222	GLY	-	linker	UNP P12493
B	223	GLY	-	linker	UNP P12493
B	224	THR	-	linker	UNP P12493
B	225	ARG	-	linker	UNP P12493
B	226	PRO	-	linker	UNP P12493
B	227	GLU	-	linker	UNP P12493
B	228	LEU	-	linker	UNP P12493
B	332	TYR	GLU	conflict	UNP P73407
B	338	GLU	ASN	conflict	UNP P73407
B	339	VAL	-	expression tag	UNP P73407
B	340	LEU	-	expression tag	UNP P73407
B	341	PHE	-	expression tag	UNP P73407
B	342	GLN	-	expression tag	UNP P73407
C	184	ALA	TRP	engineered mutation	UNP P12493
C	185	ALA	MET	engineered mutation	UNP P12493
C	220	GLY	-	linker	UNP P12493
C	221	VAL	-	linker	UNP P12493
C	222	GLY	-	linker	UNP P12493
C	223	GLY	-	linker	UNP P12493
C	224	THR	-	linker	UNP P12493
C	225	ARG	-	linker	UNP P12493
C	226	PRO	-	linker	UNP P12493
C	227	GLU	-	linker	UNP P12493
C	228	LEU	-	linker	UNP P12493
C	332	TYR	GLU	conflict	UNP P73407
C	338	GLU	ASN	conflict	UNP P73407
C	339	VAL	-	expression tag	UNP P73407
C	340	LEU	-	expression tag	UNP P73407
C	341	PHE	-	expression tag	UNP P73407
C	342	GLN	-	expression tag	UNP P73407
D	184	ALA	TRP	engineered mutation	UNP P12493
D	185	ALA	MET	engineered mutation	UNP P12493
D	220	GLY	-	linker	UNP P12493
D	221	VAL	-	linker	UNP P12493
D	222	GLY	-	linker	UNP P12493
D	223	GLY	-	linker	UNP P12493
D	224	THR	-	linker	UNP P12493

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Chain	Residue	Modelled	Actual	Comment	Reference
D	225	ARG	-	linker	UNP P12493
D	226	PRO	-	linker	UNP P12493
D	227	GLU	-	linker	UNP P12493
D	228	LEU	-	linker	UNP P12493
D	332	TYR	GLU	conflict	UNP P73407
D	338	GLU	ASN	conflict	UNP P73407
D	339	VAL	-	expression tag	UNP P73407
D	340	LEU	-	expression tag	UNP P73407
D	341	PHE	-	expression tag	UNP P73407
D	342	GLN	-	expression tag	UNP P73407
E	184	ALA	TRP	engineered mutation	UNP P12493
E	185	ALA	MET	engineered mutation	UNP P12493
E	220	GLY	-	linker	UNP P12493
E	221	VAL	-	linker	UNP P12493
E	222	GLY	-	linker	UNP P12493
E	223	GLY	-	linker	UNP P12493
E	224	THR	-	linker	UNP P12493
E	225	ARG	-	linker	UNP P12493
E	226	PRO	-	linker	UNP P12493
E	227	GLU	-	linker	UNP P12493
E	228	LEU	-	linker	UNP P12493
E	332	TYR	GLU	conflict	UNP P73407
E	338	GLU	ASN	conflict	UNP P73407
E	339	VAL	-	expression tag	UNP P73407
E	340	LEU	-	expression tag	UNP P73407
E	341	PHE	-	expression tag	UNP P73407
E	342	GLN	-	expression tag	UNP P73407
F	184	ALA	TRP	engineered mutation	UNP P12493
F	185	ALA	MET	engineered mutation	UNP P12493
F	220	GLY	-	linker	UNP P12493
F	221	VAL	-	linker	UNP P12493
F	222	GLY	-	linker	UNP P12493
F	223	GLY	-	linker	UNP P12493
F	224	THR	-	linker	UNP P12493
F	225	ARG	-	linker	UNP P12493
F	226	PRO	-	linker	UNP P12493
F	227	GLU	-	linker	UNP P12493
F	228	LEU	-	linker	UNP P12493
F	332	TYR	GLU	conflict	UNP P73407
F	338	GLU	ASN	conflict	UNP P73407
F	339	VAL	-	expression tag	UNP P73407
F	340	LEU	-	expression tag	UNP P73407

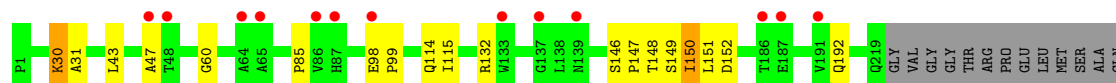
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Chain	Residue	Modelled	Actual	Comment	Reference
F	341	PHE	-	expression tag	UNP P73407
F	342	GLN	-	expression tag	UNP P73407

LYS THR ALA MET ALA GLY ILE ASP ALA ASN THR GLY ALA ASP VAL LYS THR TRP VAL ILE PRO ARG HIS GLU ASN VAL ALA VAL ALA VAL PRO ILE ASP PHE SER PRO VAL GLU VAL GLU PHE THR ARG ALA ALA GLY LEU LEU VAL LEU PHE GLN

- Molecule 1: Capsid protein p24,Carbon dioxide-concentrating mechanism protein CcmK homolog 4



SER ALA VAL SER ILE GLU THR ILE PHE PRO GLY ILE LEU ALA ALA ASP ALA ASP ALA MET VAL LYS VAL GLY THR ARG MET ALA ALA GLY SER GLN ASP

ALA ILE ASN THR GLY ALA VAL LYS THR VAL ILE ILE PRO ALA ARG PRO HIS GLU ASN VAL LYS VAL ALA VAL LEU ILE ILE ASP VAL PHE SER PRO GLU VAL GLY THR ARG PHE ARG THR TYR ILE ALA ALA ILE GLY LEU LEU VAL ASP VAL PHE GLN

- Molecule 1: Capsid protein p24,Carbon dioxide-concentrating mechanism protein CcmK homolog 4



VAL GLY SER ILE THR ILE GLY PHE PRO GLY ILE LEU ALA ALA ASP ALA ALA MET VAL LYS VAL ILE ILE PRO ARG PRO HIS ALA ASN GLU VAL VAL ALA VAL LEU ILE ILE ASP PHE SER TYR ILE ARG VAL ALA GLU PRO PHE ARG THR TYR ALA GLU LEU LEU VAL PHE GLN

ASN ARG THR GLY ALA ASP VAL TRP VAL ILE ILE PRO ARG PRO HIS ALA ASN GLU VAL VAL ALA VAL LEU ILE ILE ASP PHE SER TYR ILE ARG VAL ALA GLU PRO PHE ARG THR TYR ALA GLU LEU LEU VAL PHE GLN

- Molecule 1: Capsid protein p24,Carbon dioxide-concentrating mechanism protein CcmK homolog 4



GLN SER ALA VAL GLY ILE THR ILE PHE PRO GLY ILE LEU ALA ALA ASP ALA ASP ALA MET VAL LYS VAL ALA VAL LEU ILE ILE ASP PHE SER TYR ILE ARG VAL ALA GLU PRO PHE ARG THR TYR ALA GLU LEU LEU VAL PHE GLN

ASP ALA ILE ASN VAL ARG GLY THR LYS THR TRP VAL ILE ILE ALA PRO ARG PRO HIS GLU MET VAL LYS VAL ALA VAL LEU ILE ILE ASP PHE SER TYR ILE ARG VAL ALA GLU PRO PHE ARG THR TYR ALA GLU LEU LEU VAL PHE GLN

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.62Å 156.44Å 196.64Å 90.00° 100.35° 90.00°	Depositor
Resolution (Å)	49.75 – 7.00 49.75 – 7.00	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.75-7.00) 93.7 (49.75-7.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.10 (at 6.68Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.282 , 0.323 0.327 , 0.342	Depositor DCC
R_{free} test set	435 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	161.2	Xtriage
Anisotropy	1.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 194.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	5256	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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	0.95	0/875	1.74	11/1092 (1.0%)
1	B	0.94	0/875	1.75	12/1092 (1.1%)
1	C	0.95	0/875	1.75	11/1092 (1.0%)
1	D	0.95	0/875	1.75	11/1092 (1.0%)
1	E	0.95	0/875	1.76	12/1092 (1.1%)
1	F	0.95	0/875	1.75	11/1092 (1.0%)
All	All	0.95	0/5250	1.75	68/6552 (1.0%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	98	GLU	N-CA-C	-7.71	99.94	109.65
1	E	98	GLU	N-CA-C	-7.69	99.96	109.65
1	C	98	GLU	N-CA-C	-7.67	99.98	109.65
1	B	98	GLU	N-CA-C	-7.67	99.99	109.65
1	F	98	GLU	N-CA-C	-7.64	100.02	109.65
1	A	98	GLU	N-CA-C	-7.63	100.03	109.65
1	D	47	ALA	N-CA-C	7.63	121.26	110.50
1	A	47	ALA	N-CA-C	7.62	121.25	110.50
1	F	47	ALA	N-CA-C	7.62	121.24	110.50
1	C	47	ALA	N-CA-C	7.60	121.22	110.50
1	E	47	ALA	N-CA-C	7.58	121.19	110.50
1	B	47	ALA	N-CA-C	7.57	121.17	110.50
1	D	85	PRO	CA-C-O	6.72	129.35	121.56
1	C	85	PRO	CA-C-O	6.70	129.33	121.56
1	A	85	PRO	CA-C-O	6.69	129.32	121.56
1	F	85	PRO	CA-C-O	6.68	129.31	121.56
1	E	85	PRO	CA-C-O	6.66	129.28	121.56
1	B	85	PRO	CA-C-O	6.66	129.28	121.56
1	F	30	LYS	CA-C-O	5.78	126.05	119.18
1	B	132	ARG	CA-C-O	5.77	127.07	120.90
1	A	132	ARG	CA-C-O	5.76	127.06	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ARG	CA-C-O	5.75	127.06	120.90
1	B	30	LYS	CA-C-O	5.75	126.02	119.18
1	E	30	LYS	CA-C-O	5.74	126.01	119.18
1	D	30	LYS	CA-C-O	5.74	126.01	119.18
1	A	30	LYS	CA-C-O	5.74	126.01	119.18
1	F	132	ARG	CA-C-O	5.73	127.03	120.90
1	C	132	ARG	CA-C-O	5.70	127.00	120.90
1	C	30	LYS	CA-C-O	5.69	125.95	119.18
1	E	132	ARG	CA-C-O	5.68	126.97	120.90
1	D	60	GLY	CA-C-O	-5.54	114.55	121.53
1	C	60	GLY	CA-C-O	-5.53	114.57	121.53
1	A	60	GLY	CA-C-O	-5.51	114.58	121.53
1	B	114	GLN	N-CA-C	-5.51	105.18	111.07
1	E	114	GLN	N-CA-C	-5.50	105.19	111.07
1	E	60	GLY	CA-C-O	-5.49	114.61	121.53
1	F	60	GLY	CA-C-O	-5.48	114.63	121.53
1	C	114	GLN	N-CA-C	-5.48	105.21	111.07
1	D	114	GLN	N-CA-C	-5.47	105.22	111.07
1	A	114	GLN	N-CA-C	-5.45	105.23	111.07
1	F	114	GLN	N-CA-C	-5.44	105.25	111.07
1	B	60	GLY	CA-C-O	-5.43	114.69	121.53
1	F	115	ILE	CA-C-O	5.36	126.53	120.85
1	B	43	LEU	N-CA-C	5.34	119.42	113.01
1	E	43	LEU	N-CA-C	5.34	119.42	113.01
1	C	115	ILE	CA-C-O	5.33	126.50	120.85
1	D	43	LEU	N-CA-C	5.33	119.40	113.01
1	A	43	LEU	N-CA-C	5.32	119.39	113.01
1	A	115	ILE	CA-C-O	5.31	126.48	120.85
1	E	115	ILE	CA-C-O	5.31	126.47	120.85
1	F	43	LEU	N-CA-C	5.30	119.37	113.01
1	C	43	LEU	N-CA-C	5.30	119.37	113.01
1	B	115	ILE	CA-C-O	5.29	126.46	120.85
1	B	95	GLN	N-CA-C	-5.27	102.39	110.14
1	D	115	ILE	CA-C-O	5.24	126.41	120.85
1	D	99	PRO	CA-C-O	-5.14	115.14	121.31
1	B	99	PRO	CA-C-O	-5.11	115.17	121.31
1	A	99	PRO	CA-C-O	-5.11	115.18	121.31
1	A	192	GLN	N-CA-C	5.11	116.84	111.28
1	E	192	GLN	N-CA-C	5.08	116.81	111.28
1	C	99	PRO	CA-C-O	-5.08	115.22	121.31
1	C	192	GLN	N-CA-C	5.07	116.81	111.28
1	D	192	GLN	N-CA-C	5.07	116.80	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	99	PRO	CA-C-O	-5.06	115.24	121.31
1	F	99	PRO	CA-C-O	-5.04	115.26	121.31
1	F	192	GLN	N-CA-C	5.04	116.77	111.28
1	E	145	TYR	N-CA-C	-5.03	105.62	112.26
1	B	192	GLN	N-CA-C	5.03	116.76	111.28

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	876	0	230	7	0
1	B	876	0	230	1	0
1	C	876	0	230	3	2
1	D	876	0	230	6	0
1	E	876	0	230	2	0
1	F	876	0	230	4	0
All	All	5256	0	1380	23	2

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 3.

All (23) 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:147:PRO:CA	1:A:149:SER:N	2.40	0.84
1:F:147:PRO:O	1:F:148:THR:O	2.02	0.78
1:A:143:ARG:C	1:A:145:TYR:H	1.96	0.73
1:D:149:SER:O	1:D:151:LEU:N	2.24	0.69
1:C:146:SER:O	1:C:147:PRO:C	2.39	0.67
1:F:146:SER:O	1:F:147:PRO:C	2.41	0.62
1:A:147:PRO:CA	1:A:149:SER:H	2.13	0.62
1:A:143:ARG:O	1:A:145:TYR:N	2.35	0.59
1:A:147:PRO:CA	1:A:148:THR:C	2.75	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:SER:O	1:D:150:ILE:C	2.46	0.57
1:D:149:SER:C	1:D:151:LEU:N	2.63	0.56
1:E:149:SER:O	1:E:152:ASP:N	2.37	0.51
1:A:143:ARG:C	1:A:145:TYR:N	2.63	0.51
1:C:146:SER:O	1:C:147:PRO:O	2.30	0.49
1:F:146:SER:O	1:F:147:PRO:O	2.30	0.48
1:D:30:LYS:O	1:D:31:ALA:C	2.57	0.46
1:D:149:SER:O	1:D:152:ASP:N	2.32	0.45
1:B:30:LYS:O	1:B:31:ALA:C	2.57	0.44
1:C:30:LYS:O	1:C:31:ALA:C	2.57	0.44
1:E:30:LYS:O	1:E:31:ALA:C	2.57	0.44
1:F:30:LYS:O	1:F:31:ALA:C	2.57	0.44
1:A:30:LYS:O	1:A:31:ALA:C	2.57	0.44
1:D:149:SER:C	1:D:151:LEU:H	2.28	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:GLY:O	1:C:94:GLY:O[2_756]	1.21	0.99
1:C:7:GLN:O	1:C:89:GLY:CA[2_756]	1.82	0.38

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	217/342 (64%)	204 (94%)	8 (4%)	5 (2%)	5 28
1	B	217/342 (64%)	207 (95%)	9 (4%)	1 (0%)	24 63
1	C	217/342 (64%)	206 (95%)	8 (4%)	3 (1%)	9 40
1	D	217/342 (64%)	205 (94%)	8 (4%)	4 (2%)	6 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	217/342 (64%)	206 (95%)	10 (5%)	1 (0%)	24	63
1	F	217/342 (64%)	206 (95%)	7 (3%)	4 (2%)	6	34
All	All	1302/2052 (64%)	1234 (95%)	50 (4%)	18 (1%)	9	40

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	MET
1	A	147	PRO
1	C	146	SER
1	C	147	PRO
1	C	149	SER
1	D	146	SER
1	D	147	PRO
1	D	148	THR
1	F	147	PRO
1	F	148	THR
1	A	145	TYR
1	A	148	THR
1	D	150	ILE
1	B	147	PRO
1	F	149	SER
1	A	146	SER
1	F	146	SER
1	E	147	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	219/342 (64%)	0.32	14 (6%) 25 30	19, 33, 81, 100	0
1	B	219/342 (64%)	0.14	8 (3%) 45 43	19, 33, 81, 100	0
1	C	219/342 (64%)	0.40	16 (7%) 21 27	19, 33, 81, 100	0
1	D	219/342 (64%)	0.13	13 (5%) 28 32	19, 33, 81, 100	0
1	E	219/342 (64%)	0.16	8 (3%) 45 43	19, 33, 81, 100	0
1	F	219/342 (64%)	0.16	11 (5%) 34 35	19, 33, 81, 100	0
All	All	1314/2052 (64%)	0.22	70 (5%) 32 34	19, 33, 81, 100	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	GLY	9.9
1	C	67	GLN	5.4
1	D	98	GLU	5.4
1	C	134	ILE	5.2
1	D	65	ALA	4.3
1	D	191	VAL	4.0
1	E	137	GLY	4.0
1	D	186	THR	3.8
1	C	127	GLY	3.7
1	F	127	GLY	3.7
1	C	52	LEU	3.7
1	C	47	ALA	3.6
1	F	64	ALA	3.5
1	D	64	ALA	3.5
1	A	186	THR	3.5
1	A	187	GLU	3.5
1	A	65	ALA	3.4
1	D	187	GLU	3.4
1	E	67	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	191	VAL	3.2
1	A	22	ALA	3.1
1	F	65	ALA	3.1
1	C	11	VAL	3.1
1	B	47	ALA	3.0
1	F	191	VAL	3.0
1	B	123	PRO	3.0
1	E	191	VAL	3.0
1	B	31	ALA	2.9
1	A	98	GLU	2.9
1	C	95	GLN	2.9
1	A	10	MET	2.8
1	B	198	CYS	2.8
1	C	51	ASP	2.8
1	C	50	GLN	2.6
1	B	94	GLY	2.6
1	E	50	GLN	2.5
1	C	139	ASN	2.5
1	D	137	GLY	2.5
1	A	64	ALA	2.5
1	A	190	LEU	2.4
1	F	8	GLY	2.4
1	F	48	THR	2.4
1	C	123	PRO	2.4
1	F	58	THR	2.4
1	B	191	VAL	2.3
1	E	69	LEU	2.3
1	B	134	ILE	2.3
1	D	139	ASN	2.3
1	C	35	GLU	2.3
1	A	119	THR	2.3
1	D	87	HIS	2.3
1	A	35	GLU	2.2
1	F	50	GLN	2.2
1	F	121	ASN	2.2
1	B	185	ALA	2.2
1	F	35	GLU	2.2
1	C	1	PRO	2.1
1	D	47	ALA	2.1
1	D	133	TRP	2.1
1	D	48	THR	2.1
1	E	22	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	141	ILE	2.1
1	D	86	VAL	2.1
1	A	47	ALA	2.1
1	F	22	ALA	2.1
1	C	101	GLY	2.1
1	E	31	ALA	2.1
1	C	115	ILE	2.0
1	E	123	PRO	2.0
1	A	52	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.