Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:01 AM GMT

PDB ID	:	3GV2
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

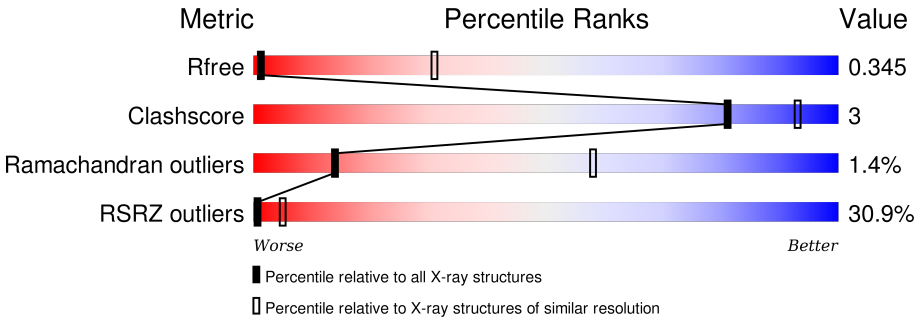
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	18% 61% 36%
1	B	342	17% 63% 36%
1	C	342	19% 62% 36%
1	D	342	21% 61% 36%
1	E	342	21% 63% 36%
1	F	342	23% 62% 36%

2 Entry composition (i)

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 Fusion protein consisting of Capsid protein p24, Linker and 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 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ALA	TRP	ENGINEERED	UNP P12497
A	185	ALA	MET	ENGINEERED	UNP P12497
A	224	THR	-	LINKER	UNP P12497
A	225	ARG	-	LINKER	UNP P12497
A	226	PRO	-	LINKER	UNP P12497
A	227	GLU	-	LINKER	UNP P12497
A	228	LEU	-	LINKER	UNP P12497
A	332	TYR	GLU	ENGINEERED	UNP P73407
A	338	GLU	-	EXPRESSION TAG	UNP P73407
A	339	VAL	-	EXPRESSION TAG	UNP P73407
A	340	LEU	-	EXPRESSION TAG	UNP P73407
A	341	PHE	-	EXPRESSION TAG	UNP P73407
A	342	GLN	-	EXPRESSION TAG	UNP P73407
B	184	ALA	TRP	ENGINEERED	UNP P12497
B	185	ALA	MET	ENGINEERED	UNP P12497
B	224	THR	-	LINKER	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
B	225	ARG	-	LINKER	UNP P12497
B	226	PRO	-	LINKER	UNP P12497
B	227	GLU	-	LINKER	UNP P12497
B	228	LEU	-	LINKER	UNP P12497
B	332	TYR	GLU	ENGINEERED	UNP P734077
B	338	GLU	-	EXPRESSION TAG	UNP P734077
B	339	VAL	-	EXPRESSION TAG	UNP P734077
B	340	LEU	-	EXPRESSION TAG	UNP P734077
B	341	PHE	-	EXPRESSION TAG	UNP P734077
B	342	GLN	-	EXPRESSION TAG	UNP P734077
C	184	ALA	TRP	ENGINEERED	UNP P12497
C	185	ALA	MET	ENGINEERED	UNP P12497
C	224	THR	-	LINKER	UNP P12497
C	225	ARG	-	LINKER	UNP P12497
C	226	PRO	-	LINKER	UNP P12497
C	227	GLU	-	LINKER	UNP P12497
C	228	LEU	-	LINKER	UNP P12497
C	332	TYR	GLU	ENGINEERED	UNP P734077
C	338	GLU	-	EXPRESSION TAG	UNP P734077
C	339	VAL	-	EXPRESSION TAG	UNP P734077
C	340	LEU	-	EXPRESSION TAG	UNP P734077
C	341	PHE	-	EXPRESSION TAG	UNP P734077
C	342	GLN	-	EXPRESSION TAG	UNP P734077
D	184	ALA	TRP	ENGINEERED	UNP P12497
D	185	ALA	MET	ENGINEERED	UNP P12497
D	224	THR	-	LINKER	UNP P12497
D	225	ARG	-	LINKER	UNP P12497
D	226	PRO	-	LINKER	UNP P12497
D	227	GLU	-	LINKER	UNP P12497
D	228	LEU	-	LINKER	UNP P12497
D	332	TYR	GLU	ENGINEERED	UNP P734077
D	338	GLU	-	EXPRESSION TAG	UNP P734077
D	339	VAL	-	EXPRESSION TAG	UNP P734077
D	340	LEU	-	EXPRESSION TAG	UNP P734077
D	341	PHE	-	EXPRESSION TAG	UNP P734077
D	342	GLN	-	EXPRESSION TAG	UNP P734077
E	184	ALA	TRP	ENGINEERED	UNP P12497
E	185	ALA	MET	ENGINEERED	UNP P12497
E	224	THR	-	LINKER	UNP P12497
E	225	ARG	-	LINKER	UNP P12497
E	226	PRO	-	LINKER	UNP P12497
E	227	GLU	-	LINKER	UNP P12497

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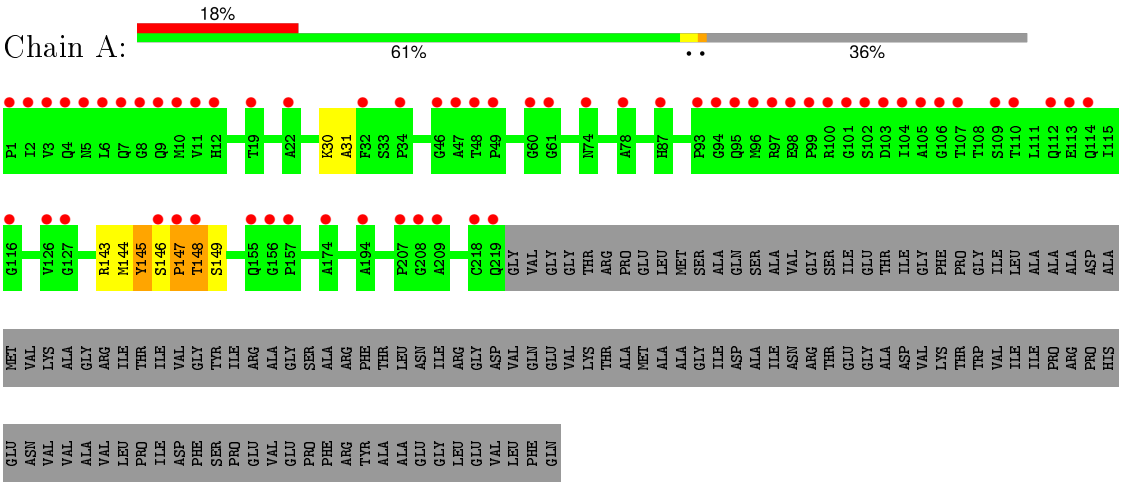
Chain	Residue	Modelled	Actual	Comment	Reference
E	228	LEU	-	LINKER	UNP P12497
E	332	TYR	GLU	ENGINEERED	UNP P734077
E	338	GLU	-	EXPRESSION TAG	UNP P734077
E	339	VAL	-	EXPRESSION TAG	UNP P734077
E	340	LEU	-	EXPRESSION TAG	UNP P734077
E	341	PHE	-	EXPRESSION TAG	UNP P734077
E	342	GLN	-	EXPRESSION TAG	UNP P734077
F	184	ALA	TRP	ENGINEERED	UNP P12497
F	185	ALA	MET	ENGINEERED	UNP P12497
F	224	THR	-	LINKER	UNP P12497
F	225	ARG	-	LINKER	UNP P12497
F	226	PRO	-	LINKER	UNP P12497
F	227	GLU	-	LINKER	UNP P12497
F	228	LEU	-	LINKER	UNP P12497
F	332	TYR	GLU	ENGINEERED	UNP P734077
F	338	GLU	-	EXPRESSION TAG	UNP P734077
F	339	VAL	-	EXPRESSION TAG	UNP P734077
F	340	LEU	-	EXPRESSION TAG	UNP P734077
F	341	PHE	-	EXPRESSION TAG	UNP P734077
F	342	GLN	-	EXPRESSION TAG	UNP P734077

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

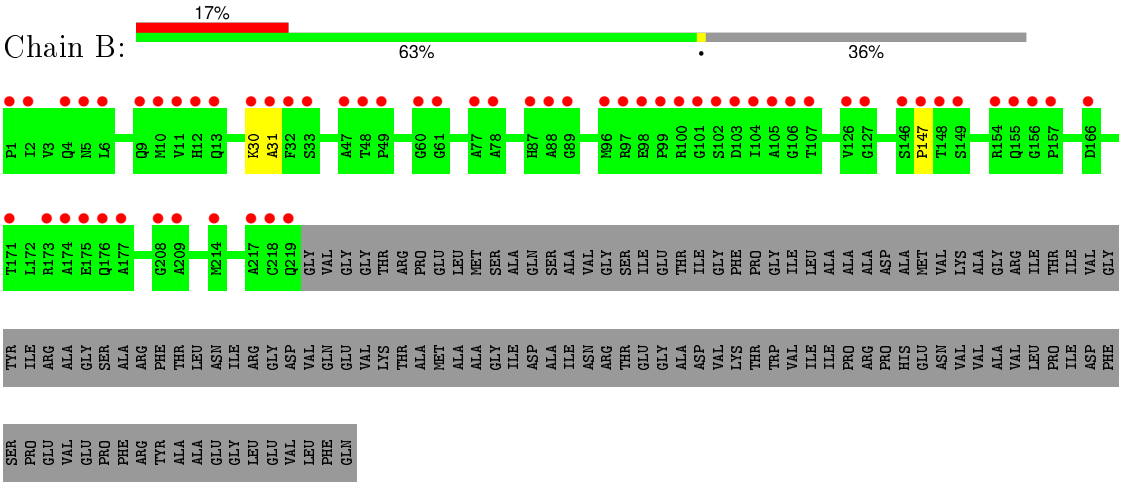
• Molecule 1: Fusion protein consisting of Capsid protein p24, Linker and Carbon dioxide-concen trating mechanism protein ccmK homolog 4

Chain A:



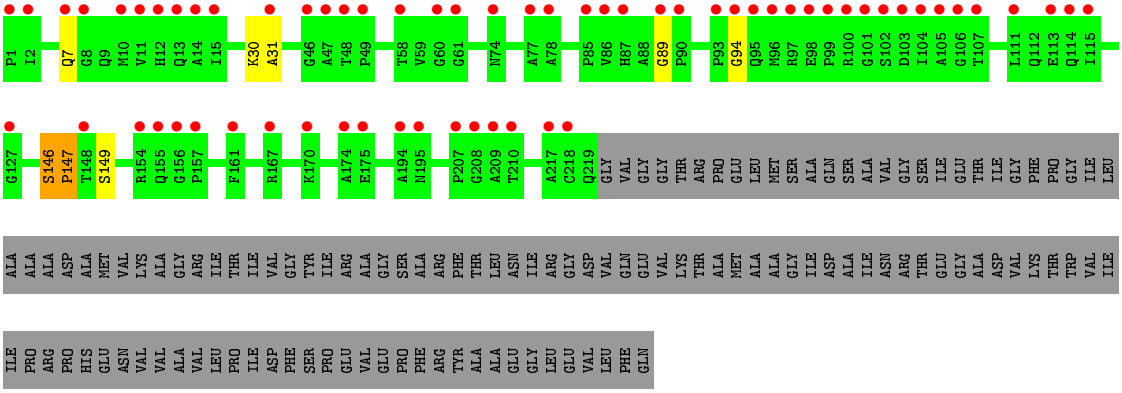
• Molecule 1: Fusion protein consisting of Capsid protein p24, Linker and Carbon dioxide-concen trating mechanism protein ccmK homolog 4

Chain B:



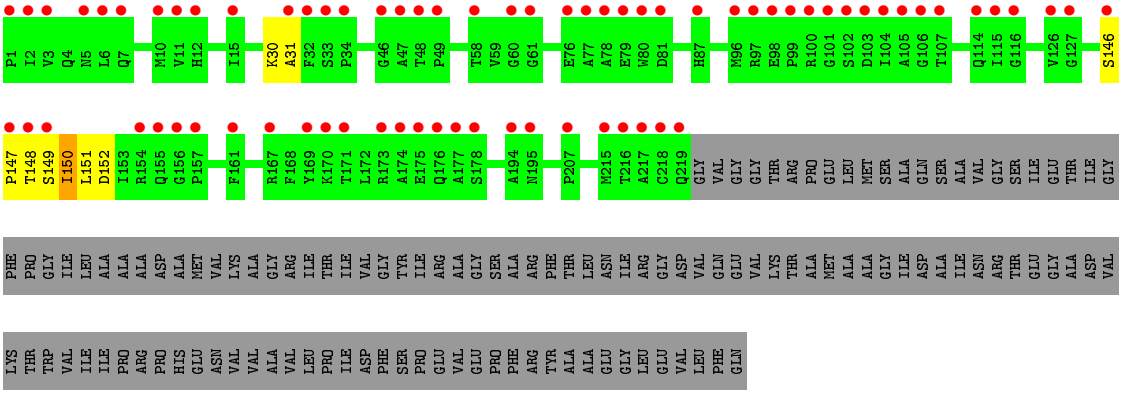
• Molecule 1: Fusion protein consisting of Capsid protein p24, Linker and Carbon dioxide-concen trating mechanism protein ccmK homolog 4

Chain C:



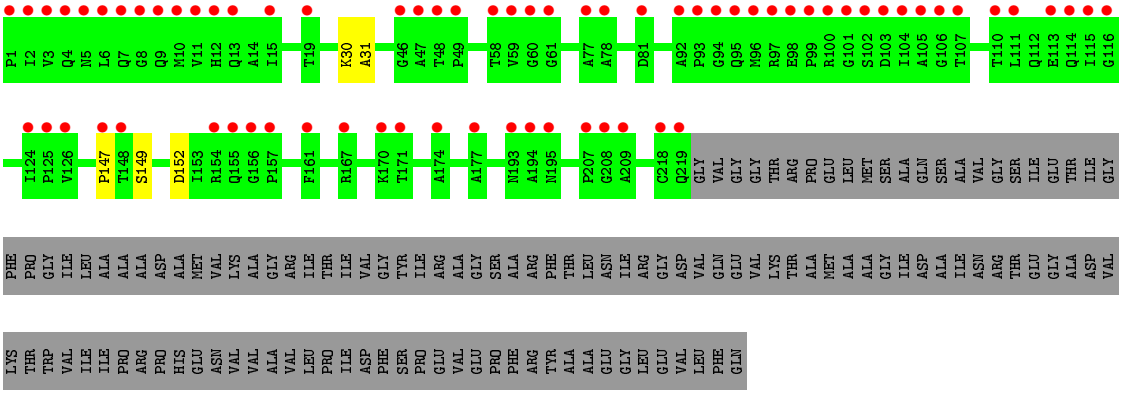
• Molecule 1: Fusion protein consisting of Capsid protein p24, Linker and Carbon dioxide-concen trating mechanism protein ccmK homolog 4

Chain D:



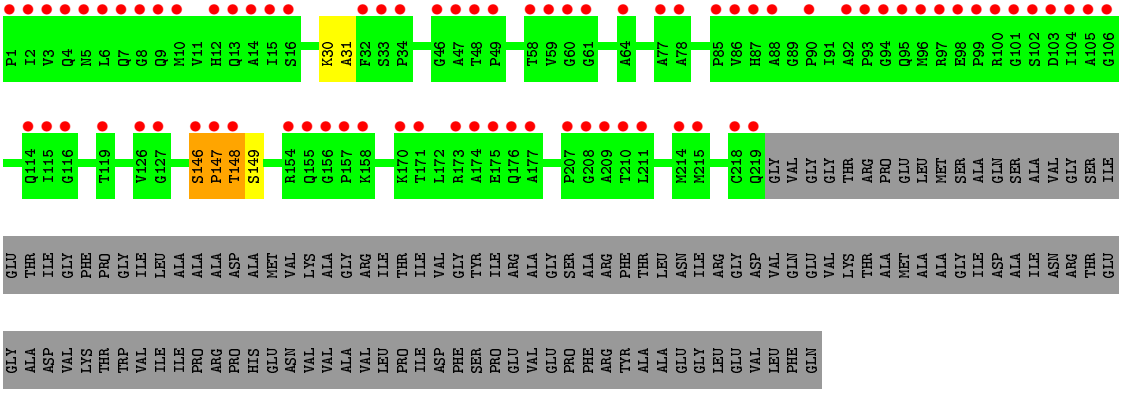
• Molecule 1: Fusion protein consisting of Capsid protein p24, Linker and Carbon dioxide-concen trating mechanism protein ccmK homolog 4

Chain E:



• Molecule 1: Fusion protein consisting of Capsid protein p24, Linker and Carbon dioxide-concen trating mechanism protein ccmK homolog 4

Chain F:


P1 I2 V3 Q4 N5 L6 Q7 G8 Q9 M10 V11 H12 Q13 A14 I15 S16 K30 A31 F32 S33 P34 G46 A47 T48 P49 T58 V59 G60 G61 A64 A77 A78 P85 V86 H87 A88 G89 P90 I91 A92 P93 G94 Q95 N96 R97 E98 P99 R100 G101 S102 D103 T104 A105 G106
Q114 I115 G116 T119 V126 G127 S146 P147 T148 S149 R154 Q155 G156 P157 K158 K170 T171 L172 R173 A174 E175 Q176 A177 P207 G208 A209 T210 L211 M214 M215 C218 Q219 GLY VAL GLY GLY THR ARG PRO GLU LEU MET SER ALA GLN SER ALA VAL GLY SER ILE
GLU THR ILE GLY PHE PRO GLY ILE LEU ALA ALA ALA ASP ALA MET VAL LYS ALA GLY ARG ILE THR ILE VAL GLY TYR ILE ARG ALA GLY SER ALA ARG PHE THR LEU ASN ILE ARG GLY ASP VAL GLN GLU VAL LYS THR ALA MET ALA ALA GLY ILE ASP ALA ILE ASN ARG THR GLU
GLY ALA ASP VAL LYS THR TRP VAL ILE ILE PRO ARG PRO HIS GLU ASN VAL VAL ALA VAL LEU PRO ILE ASP PHE SER PRO GLU VAL GLU PRO PHE ARG TYR ALA ALA GLU GLY LEU GLU VAL LEU PHE GLN

4 Data and refinement statistics (i)

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 – 6.95	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.75-7.00) 81.2 (49.75-6.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.10 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.282 , 0.323 0.301 , 0.345	Depositor DCC
R_{free} test set	409 reflections (10.08%)	DCC
Wilson B-factor (Å^2)	161.2	Xtriage
Anisotropy	1.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 341.8	EDS
Estimated twinning fraction	0.116 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 4325 reflections (0.046%)	Xtriage
F_o,F_c correlation	0.71	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.57	0/875	1.02	0/1092
1	B	0.56	0/875	1.02	0/1092
1	C	0.57	0/875	1.02	0/1092
1	D	0.57	0/875	1.03	0/1092
1	E	0.57	0/875	1.03	0/1092
1	F	0.57	0/875	1.03	0/1092
All	All	0.57	0/5250	1.02	0/6552

There are no bond length outliers.

There are no bond angle outliers.

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	876	0	230	7	0
1	B	876	0	230	1	0
1	C	876	0	230	3	2
1	D	876	0	230	5	0
1	E	876	0	230	2	0
1	F	876	0	230	4	0
All	All	5256	0	1380	22	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 (22) 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:D:149:SER:O	1:D:151:LEU:N	2.24	0.69
1:A:143:ARG:C	1:A:145:TYR:H	1.96	0.68
1:A:147:PRO:CA	1:A:149:SER:H	2.13	0.62
1:C:146:SER:O	1:C:147:PRO:C	2.39	0.62
1:A:143:ARG:O	1:A:145:TYR:N	2.35	0.59
1:F:146:SER:O	1:F:147:PRO:C	2.41	0.58
1:A:147:PRO:CA	1:A:148:THR:C	2.75	0.53
1:D:149:SER:O	1:D:150:ILE:C	2.46	0.52
1:D:149:SER:C	1:D:151:LEU:N	2.63	0.51
1:E:149:SER:O	1:E:152:ASP:N	2.37	0.51
1:F:146:SER:O	1:F:147:PRO:O	2.30	0.49
1:C:146:SER:O	1:C:147:PRO:O	2.30	0.49
1:A:143:ARG:C	1:A:145:TYR:N	2.63	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	0.42
1:A:30:LYS:O	1:A:31:ALA:C	2.57	0.42
1:C:30:LYS:O	1:C:31:ALA:C	2.57	0.42
1:D:30:LYS:O	1:D:31:ALA:C	2.57	0.41
1:F:30:LYS:O	1:F:31:ALA:C	2.57	0.40
1:E:30:LYS:O	1:E:31:ALA:C	2.57	0.40

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%)	8 48
1	B	217/342 (64%)	207 (95%)	9 (4%)	1 (0%)	34 77
1	C	217/342 (64%)	206 (95%)	8 (4%)	3 (1%)	14 58
1	D	217/342 (64%)	205 (94%)	8 (4%)	4 (2%)	11 53
1	E	217/342 (64%)	206 (95%)	10 (5%)	1 (0%)	34 77
1	F	217/342 (64%)	206 (95%)	7 (3%)	4 (2%)	11 53
All	All	1302/2052 (64%)	1234 (95%)	50 (4%)	18 (1%)	14 58

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	1.47	61 (27%) 1 5	19, 33, 81, 100	0
1	B	219/342 (64%)	1.39	59 (26%) 1 5	19, 33, 81, 100	0
1	C	219/342 (64%)	1.64	64 (29%) 1 5	19, 33, 81, 100	0
1	D	219/342 (64%)	1.60	72 (32%) 0 5	19, 33, 81, 100	0
1	E	219/342 (64%)	1.59	71 (32%) 1 5	19, 33, 81, 100	0
1	F	219/342 (64%)	1.78	79 (36%) 0 4	19, 33, 81, 100	0
All	All	1314/2052 (64%)	1.58	406 (30%) 1 5	19, 33, 81, 100	0

All (406) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	GLY	12.8
1	A	99	PRO	11.5
1	B	148	THR	9.2
1	A	98	GLU	9.2
1	F	7	GLN	9.1
1	D	148	THR	8.7
1	D	105	ALA	8.5
1	E	105	ALA	8.5
1	C	1	PRO	8.4
1	A	97	ARG	8.4
1	A	100	ARG	8.3
1	E	104	ILE	8.2
1	E	101	GLY	8.0
1	D	101	GLY	8.0
1	C	105	ALA	7.8
1	C	2	ILE	7.8
1	C	95	GLN	7.8
1	F	94	GLY	7.7
1	D	99	PRO	7.6

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Mol	Chain	Res	Type	RSRZ
1	B	99	PRO	7.5
1	A	101	GLY	7.5
1	D	98	GLU	7.5
1	B	101	GLY	7.4
1	B	105	ALA	7.4
1	F	8	GLY	7.4
1	F	5	ASN	7.3
1	B	100	ARG	7.2
1	D	100	ARG	7.1
1	C	101	GLY	7.0
1	D	97	ARG	7.0
1	E	103	ASP	7.0
1	E	47	ALA	7.0
1	C	155	GLN	6.9
1	E	100	ARG	6.8
1	F	105	ALA	6.8
1	F	6	LEU	6.6
1	F	98	GLU	6.6
1	F	93	PRO	6.6
1	C	47	ALA	6.5
1	D	104	ILE	6.5
1	A	9	GLN	6.5
1	C	99	PRO	6.4
1	A	105	ALA	6.3
1	D	147	PRO	6.3
1	F	95	GLN	6.3
1	B	104	ILE	6.1
1	E	99	PRO	6.1
1	A	104	ILE	6.1
1	E	98	GLU	6.1
1	A	47	ALA	6.1
1	C	174	ALA	6.1
1	D	47	ALA	6.0
1	C	12	HIS	6.0
1	C	46	GLY	5.9
1	F	1	PRO	5.9
1	E	102	SER	5.9
1	B	147	PRO	5.9
1	D	177	ALA	5.9
1	C	104	ILE	5.8
1	C	98	GLU	5.8
1	E	48	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	46	GLY	5.7
1	C	100	ARG	5.7
1	B	218	CYS	5.7
1	A	2	ILE	5.6
1	D	174	ALA	5.6
1	A	8	GLY	5.6
1	B	155	GLN	5.5
1	E	1	PRO	5.4
1	C	209	ALA	5.4
1	F	99	PRO	5.4
1	F	101	GLY	5.4
1	F	96	MET	5.3
1	A	10	MET	5.3
1	B	12	HIS	5.3
1	F	127	GLY	5.3
1	D	155	GLN	5.1
1	A	7	GLN	5.1
1	E	208	GLY	5.1
1	F	9	GLN	5.1
1	D	2	ILE	5.1
1	A	5	ASN	5.1
1	F	157	PRO	5.1
1	C	11	VAL	5.0
1	A	155	GLN	5.0
1	E	194	ALA	5.0
1	D	154	ARG	4.9
1	B	174	ALA	4.9
1	A	1	PRO	4.9
1	F	47	ALA	4.8
1	D	175	GLU	4.8
1	E	97	ARG	4.8
1	C	103	ASP	4.7
1	C	97	ARG	4.7
1	A	96	MET	4.7
1	C	13	GLN	4.7
1	E	10	MET	4.7
1	E	106	GLY	4.7
1	F	2	ILE	4.6
1	D	96	MET	4.6
1	F	155	GLN	4.6
1	E	147	PRO	4.6
1	E	2	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	4	GLN	4.6
1	A	106	GLY	4.6
1	E	155	GLN	4.6
1	F	218	CYS	4.6
1	A	46	GLY	4.6
1	B	1	PRO	4.6
1	B	98	GLU	4.6
1	B	208	GLY	4.5
1	A	102	SER	4.5
1	C	154	ARG	4.5
1	E	5	ASN	4.5
1	C	127	GLY	4.5
1	B	157	PRO	4.5
1	D	219	GLN	4.4
1	E	11	VAL	4.4
1	F	156	GLY	4.4
1	F	100	ARG	4.4
1	F	33	SER	4.4
1	A	157	PRO	4.4
1	C	106	GLY	4.3
1	F	104	ILE	4.3
1	D	1	PRO	4.3
1	D	173	ARG	4.3
1	D	48	THR	4.3
1	F	10	MET	4.3
1	D	156	GLY	4.3
1	D	77	ALA	4.3
1	E	114	GLN	4.3
1	F	87	HIS	4.3
1	D	102	SER	4.3
1	D	171	THR	4.2
1	E	60	GLY	4.2
1	C	49	PRO	4.2
1	A	147	PRO	4.2
1	A	11	VAL	4.2
1	D	60	GLY	4.2
1	F	46	GLY	4.1
1	F	174	ALA	4.1
1	B	47	ALA	4.1
1	B	106	GLY	4.1
1	B	102	SER	4.1
1	A	61	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	12	HIS	4.1
1	E	126	VAL	4.1
1	A	48	THR	4.1
1	B	209	ALA	4.0
1	A	3	VAL	4.0
1	C	102	SER	4.0
1	E	9	GLN	4.0
1	E	94	GLY	4.0
1	E	174	ALA	4.0
1	A	148	THR	4.0
1	C	10	MET	4.0
1	F	97	ARG	3.9
1	E	148	THR	3.9
1	D	78	ALA	3.9
1	E	171	THR	3.9
1	F	48	THR	3.9
1	A	103	ASP	3.9
1	D	157	PRO	3.9
1	F	106	GLY	3.9
1	F	60	GLY	3.8
1	C	208	GLY	3.8
1	A	4	GLN	3.8
1	C	93	PRO	3.8
1	C	96	MET	3.8
1	D	11	VAL	3.8
1	D	176	GLN	3.8
1	F	208	GLY	3.8
1	E	46	GLY	3.7
1	C	14	ALA	3.7
1	E	96	MET	3.7
1	E	157	PRO	3.7
1	C	61	GLY	3.7
1	F	171	THR	3.7
1	C	156	GLY	3.7
1	D	218	CYS	3.6
1	D	107	THR	3.6
1	B	156	GLY	3.6
1	E	4	GLN	3.6
1	F	92	ALA	3.6
1	D	106	GLY	3.6
1	F	61	GLY	3.6
1	E	3	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	5	ASN	3.6
1	A	114	GLN	3.6
1	D	33	SER	3.5
1	F	15	ILE	3.5
1	B	176	GLN	3.5
1	C	148	THR	3.5
1	A	156	GLY	3.5
1	B	88	ALA	3.5
1	E	95	GLN	3.5
1	C	194	ALA	3.5
1	F	34	PRO	3.5
1	B	31	ALA	3.4
1	D	79	GLU	3.4
1	D	61	GLY	3.4
1	A	107	THR	3.4
1	C	87	HIS	3.4
1	B	32	PHE	3.4
1	B	49	PRO	3.4
1	E	113	GLU	3.4
1	C	157	PRO	3.4
1	B	127	GLY	3.4
1	A	49	PRO	3.4
1	F	103	ASP	3.4
1	F	146	SER	3.4
1	B	219	GLN	3.3
1	F	175	GLU	3.3
1	B	103	ASP	3.3
1	E	209	ALA	3.3
1	B	154	ARG	3.3
1	B	11	VAL	3.3
1	D	167	ARG	3.3
1	B	60	GLY	3.3
1	A	95	GLN	3.3
1	A	127	GLY	3.3
1	B	48	THR	3.3
1	E	156	GLY	3.2
1	C	58	THR	3.2
1	A	94	GLY	3.2
1	E	78	ALA	3.2
1	F	126	VAL	3.2
1	E	61	GLY	3.2
1	F	154	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	6	LEU	3.2
1	E	219	GLN	3.2
1	B	177	ALA	3.2
1	C	48	THR	3.2
1	D	34	PRO	3.2
1	A	6	LEU	3.2
1	B	175	GLU	3.2
1	E	77	ALA	3.2
1	D	5	ASN	3.2
1	D	146	SER	3.2
1	C	114	GLN	3.2
1	B	87	HIS	3.1
1	B	10	MET	3.1
1	F	16	SER	3.1
1	F	49	PRO	3.1
1	B	61	GLY	3.1
1	A	209	ALA	3.1
1	D	103	ASP	3.1
1	A	219	GLN	3.1
1	E	7	GLN	3.1
1	E	170	LYS	3.1
1	F	219	GLN	3.1
1	B	33	SER	3.0
1	F	102	SER	3.0
1	E	58	THR	3.0
1	A	208	GLY	3.0
1	F	32	PHE	3.0
1	C	86	VAL	3.0
1	C	15	ILE	3.0
1	D	170	LYS	3.0
1	D	31	ALA	3.0
1	D	194	ALA	3.0
1	F	177	ALA	3.0
1	F	88	ALA	2.9
1	D	114	GLN	2.9
1	E	207	PRO	2.9
1	A	194	ALA	2.9
1	E	49	PRO	2.9
1	F	86	VAL	2.9
1	F	58	THR	2.9
1	E	154	ARG	2.9
1	A	60	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	12	HIS	2.8
1	D	215	MET	2.8
1	F	148	THR	2.8
1	D	81	ASP	2.8
1	C	170	LYS	2.8
1	E	124	ILE	2.8
1	A	87	HIS	2.8
1	C	78	ALA	2.8
1	E	15	ILE	2.8
1	F	78	ALA	2.8
1	B	149	SER	2.7
1	B	89	GLY	2.7
1	D	217	ALA	2.7
1	E	115	ILE	2.7
1	B	2	ILE	2.7
1	A	126	VAL	2.7
1	F	209	ALA	2.7
1	D	178	SER	2.7
1	F	13	GLN	2.7
1	B	77	ALA	2.7
1	A	93	PRO	2.7
1	E	107	THR	2.7
1	D	3	VAL	2.7
1	D	126	VAL	2.7
1	B	146	SER	2.7
1	F	14	ALA	2.7
1	E	167	ARG	2.7
1	D	32	PHE	2.7
1	C	60	GLY	2.7
1	C	85	PRO	2.7
1	D	195	ASN	2.6
1	E	13	GLN	2.6
1	E	195	ASN	2.6
1	B	13	GLN	2.6
1	D	6	LEU	2.6
1	E	116	GLY	2.6
1	D	169	TYR	2.6
1	E	218	CYS	2.6
1	B	166	ASP	2.6
1	C	107	THR	2.6
1	D	7	GLN	2.6
1	F	116	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	59	VAL	2.6
1	D	216	THR	2.6
1	A	113	GLU	2.6
1	A	146	SER	2.6
1	E	161	PHE	2.6
1	B	217	ALA	2.6
1	B	97	ARG	2.6
1	D	15	ILE	2.5
1	E	193	ASN	2.5
1	C	8	GLY	2.5
1	F	119	THR	2.5
1	C	90	PRO	2.5
1	F	3	VAL	2.5
1	C	175	GLU	2.5
1	D	10	MET	2.5
1	D	58	THR	2.5
1	B	4	GLN	2.5
1	B	126	VAL	2.5
1	F	158	LYS	2.5
1	F	215	MET	2.5
1	C	195	ASN	2.5
1	A	112	GLN	2.5
1	C	210	THR	2.4
1	B	6	LEU	2.4
1	C	77	ALA	2.4
1	D	149	SER	2.4
1	D	49	PRO	2.4
1	F	59	VAL	2.4
1	D	207	PRO	2.4
1	E	8	GLY	2.4
1	C	74	ASN	2.4
1	F	210	THR	2.4
1	A	110	THR	2.4
1	A	174	ALA	2.4
1	F	77	ALA	2.4
1	A	218	CYS	2.4
1	B	173	ARG	2.4
1	C	31	ALA	2.4
1	B	9	GLN	2.3
1	F	170	LYS	2.3
1	C	7	GLN	2.3
1	A	34	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	93	PRO	2.3
1	D	127	GLY	2.3
1	D	87	HIS	2.3
1	E	111	LEU	2.3
1	C	167	ARG	2.3
1	A	109	SER	2.3
1	C	111	LEU	2.3
1	B	30	LYS	2.3
1	A	32	PHE	2.3
1	B	171	THR	2.3
1	A	207	PRO	2.3
1	C	161	PHE	2.2
1	A	12	HIS	2.2
1	F	214	MET	2.2
1	F	12	HIS	2.2
1	F	85	PRO	2.2
1	C	113	GLU	2.2
1	F	211	LEU	2.2
1	E	92	ALA	2.2
1	C	218	CYS	2.2
1	A	19	THR	2.2
1	B	214	MET	2.2
1	F	176	GLN	2.2
1	A	116	GLY	2.2
1	F	114	GLN	2.2
1	B	107	THR	2.1
1	E	125	PRO	2.1
1	F	90	PRO	2.1
1	A	78	ALA	2.1
1	E	81	ASP	2.1
1	E	110	THR	2.1
1	C	115	ILE	2.1
1	C	89	GLY	2.1
1	D	161	PHE	2.1
1	F	115	ILE	2.1
1	F	173	ARG	2.1
1	A	22	ALA	2.1
1	C	217	ALA	2.1
1	B	78	ALA	2.1
1	E	19	THR	2.1
1	D	76	GLU	2.1
1	D	116	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	177	ALA	2.1
1	F	147	PRO	2.0
1	D	115	ILE	2.0
1	F	207	PRO	2.0
1	A	74	ASN	2.0
1	D	80	TRP	2.0
1	B	96	MET	2.0
1	F	64	ALA	2.0
1	C	207	PRO	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 carbohydrates 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.