Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:57 PM GMT

PDB ID	:	5EJK
Title	:	Crystal structure of the Rous sarcoma virus intasome
Authors	:	Yin, Z.; Shi, K.; Banerjee, S.; Aihara, H.
Deposited on	:	2015-11-02
Resolution	:	3.80 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:

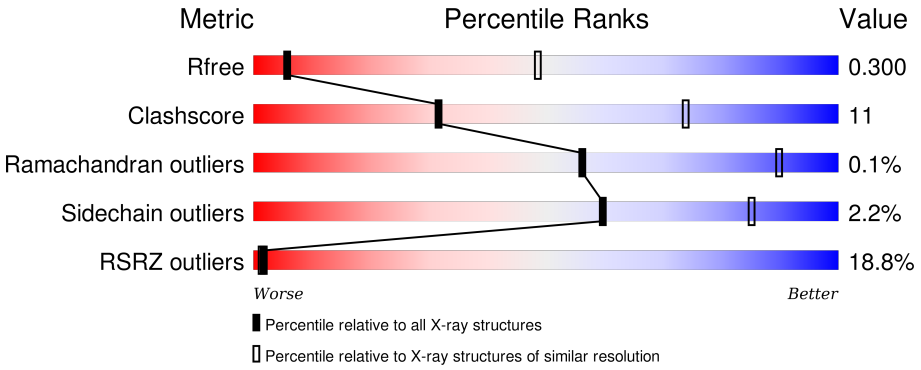
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 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	270	17% 74% 24% •
1	B	270	16% 77% 17% 6%
1	C	270	14% 70% 23% • 5%
1	D	270	23% 70% 22% • 7%
1	E	270	9% 72% 26% •

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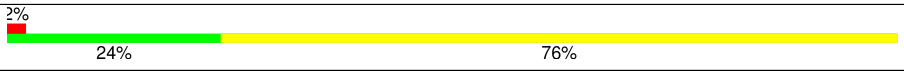
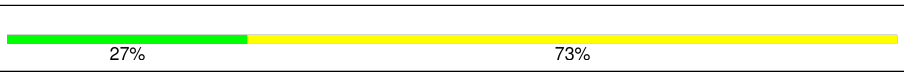
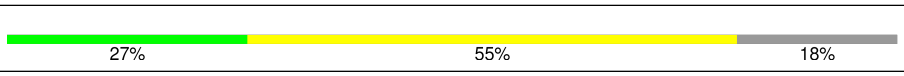
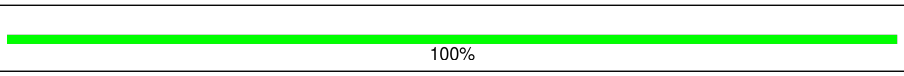
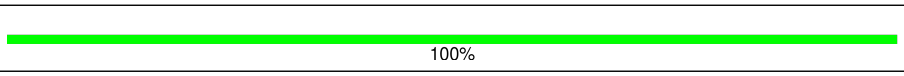
Mol	Chain	Length	Quality of chain
1	F	270	
1	G	270	
1	H	270	
2	I	42	
2	L	42	
3	J	22	
3	M	22	
4	K	8	
4	N	8	
5	k	8	
5	n	8	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19335 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 Gag-Pro-Pol polyprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	Se	0	0	0
			2099	1316	396	373	3	11			
1	B	253	Total	C	N	O	S	Se	0	0	0
			1993	1252	375	352	3	11			
1	C	256	Total	C	N	O	S	Se	0	0	0
			2009	1262	378	355	3	11			
1	D	250	Total	C	N	O	S	Se	0	0	0
			1967	1235	372	346	3	11			
1	E	269	Total	C	N	O	S	Se	0	0	0
			2099	1316	396	373	3	11			
1	F	254	Total	C	N	O	S	Se	0	0	0
			1997	1254	376	353	3	11			
1	G	250	Total	C	N	O	S	Se	0	0	0
			1972	1241	372	345	3	11			
1	H	263	Total	C	N	O	S	Se	0	0	0
			2058	1290	389	365	3	11			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	SER	CYS	engineered mutation	UNP P03354
A	112	MSE	LEU	engineered mutation	UNP P03354
A	135	MSE	LEU	engineered mutation	UNP P03354
A	162	MSE	LEU	engineered mutation	UNP P03354
A	163	MSE	LEU	engineered mutation	UNP P03354
A	166	LYS	ARG	conflict	UNP P03354
A	188	MSE	LEU	engineered mutation	UNP P03354
A	189	MSE	LEU	engineered mutation	UNP P03354
B	23	SER	CYS	engineered mutation	UNP P03354
B	112	MSE	LEU	engineered mutation	UNP P03354
B	135	MSE	LEU	engineered mutation	UNP P03354
B	162	MSE	LEU	engineered mutation	UNP P03354
B	163	MSE	LEU	engineered mutation	UNP P03354

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Chain	Residue	Modelled	Actual	Comment	Reference
B	166	LYS	ARG	conflict	UNP P03354
B	188	MSE	LEU	engineered mutation	UNP P03354
B	189	MSE	LEU	engineered mutation	UNP P03354
C	23	SER	CYS	engineered mutation	UNP P03354
C	112	MSE	LEU	engineered mutation	UNP P03354
C	135	MSE	LEU	engineered mutation	UNP P03354
C	162	MSE	LEU	engineered mutation	UNP P03354
C	163	MSE	LEU	engineered mutation	UNP P03354
C	166	LYS	ARG	conflict	UNP P03354
C	188	MSE	LEU	engineered mutation	UNP P03354
C	189	MSE	LEU	engineered mutation	UNP P03354
D	23	SER	CYS	engineered mutation	UNP P03354
D	112	MSE	LEU	engineered mutation	UNP P03354
D	135	MSE	LEU	engineered mutation	UNP P03354
D	162	MSE	LEU	engineered mutation	UNP P03354
D	163	MSE	LEU	engineered mutation	UNP P03354
D	166	LYS	ARG	conflict	UNP P03354
D	188	MSE	LEU	engineered mutation	UNP P03354
D	189	MSE	LEU	engineered mutation	UNP P03354
E	23	SER	CYS	engineered mutation	UNP P03354
E	112	MSE	LEU	engineered mutation	UNP P03354
E	135	MSE	LEU	engineered mutation	UNP P03354
E	162	MSE	LEU	engineered mutation	UNP P03354
E	163	MSE	LEU	engineered mutation	UNP P03354
E	166	LYS	ARG	conflict	UNP P03354
E	188	MSE	LEU	engineered mutation	UNP P03354
E	189	MSE	LEU	engineered mutation	UNP P03354
F	23	SER	CYS	engineered mutation	UNP P03354
F	112	MSE	LEU	engineered mutation	UNP P03354
F	135	MSE	LEU	engineered mutation	UNP P03354
F	162	MSE	LEU	engineered mutation	UNP P03354
F	163	MSE	LEU	engineered mutation	UNP P03354
F	166	LYS	ARG	conflict	UNP P03354
F	188	MSE	LEU	engineered mutation	UNP P03354
F	189	MSE	LEU	engineered mutation	UNP P03354
G	23	SER	CYS	engineered mutation	UNP P03354
G	112	MSE	LEU	engineered mutation	UNP P03354
G	135	MSE	LEU	engineered mutation	UNP P03354
G	162	MSE	LEU	engineered mutation	UNP P03354
G	163	MSE	LEU	engineered mutation	UNP P03354
G	166	LYS	ARG	conflict	UNP P03354
G	188	MSE	LEU	engineered mutation	UNP P03354

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Chain	Residue	Modelled	Actual	Comment	Reference
G	189	MSE	LEU	engineered mutation	UNP P03354
H	23	SER	CYS	engineered mutation	UNP P03354
H	112	MSE	LEU	engineered mutation	UNP P03354
H	135	MSE	LEU	engineered mutation	UNP P03354
H	162	MSE	LEU	engineered mutation	UNP P03354
H	163	MSE	LEU	engineered mutation	UNP P03354
H	166	LYS	ARG	conflict	UNP P03354
H	188	MSE	LEU	engineered mutation	UNP P03354
H	189	MSE	LEU	engineered mutation	UNP P03354

- Molecule 2 is a DNA chain called RSV Integrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	42	Total	C	N	O	P	0	0	0
			869	413	178	237	41			
2	L	38	Total	C	N	O	P	0	0	0
			787	373	161	215	38			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*AP*TP*GP*TP*TP*GP*TP*CP*TP*TP*AP*TP*GP*CP*AP*AP*TP*AP*CP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	22	Total	C	N	O	P	0	0	0
			445	216	75	133	21			
3	M	18	Total	C	N	O	P	0	0	0
			366	178	62	109	17			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*TP*TP*CP*TP*CP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	8	Total	C	N	O	P	0	0	0
			154	77	19	51	7			
4	N	8	Total	C	N	O	P	0	0	0
			154	77	19	51	7			

- Molecule 5 is a DNA chain called DNA (5'-D(*AP*GP*TP*GP*TP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	8	Total	C	N	O	P	0	0	0
			161	79	26	49	7			
5	n	8	Total	C	N	O	P	0	0	0
			161	79	26	49	7			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Zn 1 1	0	0
6	D	1	Total Zn 1 1	0	0
6	E	1	Total Zn 1 1	0	0
6	H	1	Total Zn 1 1	0	0
6	B	1	Total Zn 1 1	0	0
6	C	1	Total Zn 1 1	0	0
6	A	1	Total Zn 1 1	0	0
6	F	1	Total Zn 1 1	0	0

- Molecule 7 is TUNGSTEN ION (three-letter code: W) (formula: W).

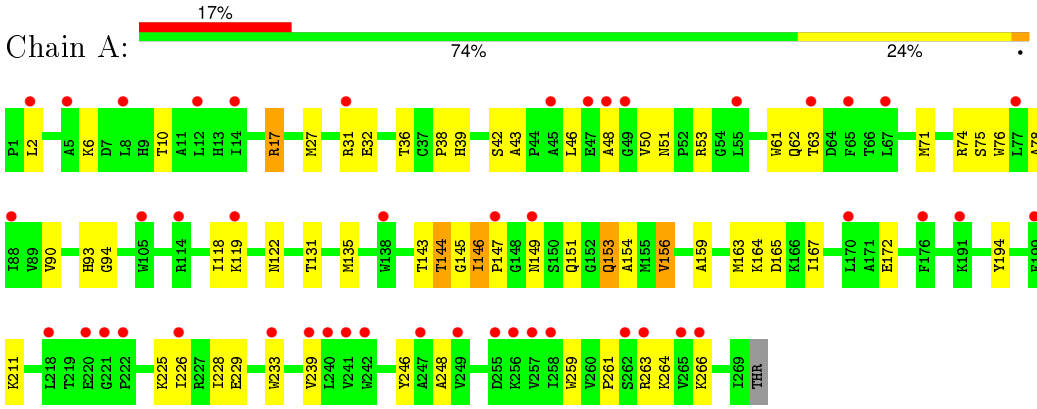
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total W 1 1	0	0
7	B	20	Total W 20 20	0	0
7	A	4	Total W 4 4	1	0
7	F	11	Total W 11 11	0	0

3 Residue-property plots (i)

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.

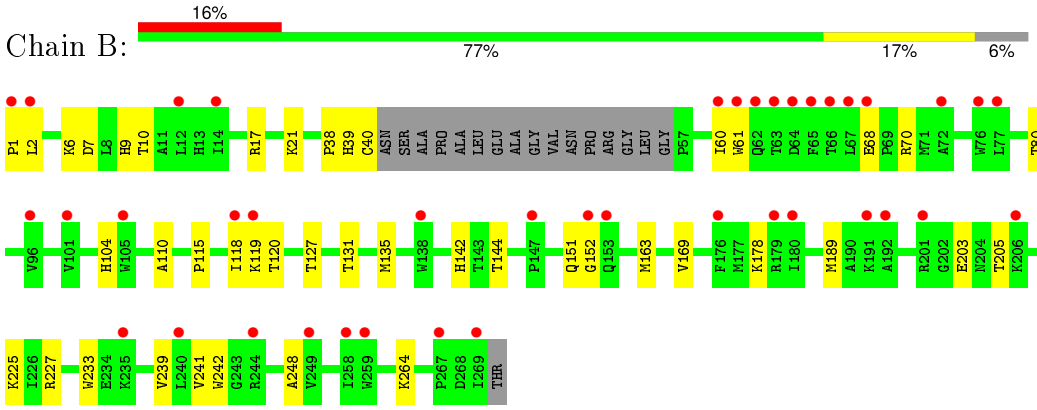
- Molecule 1: Gag-Pro-Pol polyprotein

Chain A:



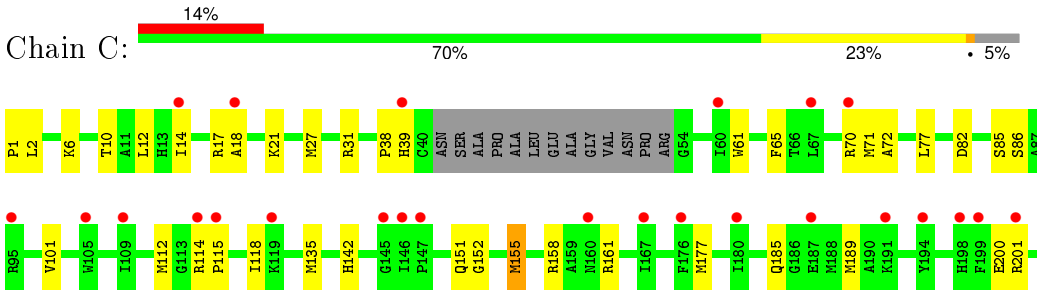
- Molecule 1: Gag-Pro-Pol polyprotein

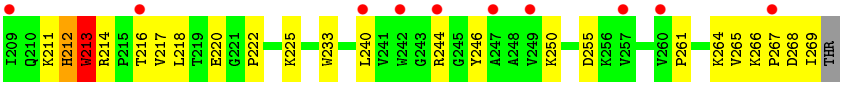
Chain B:



- Molecule 1: Gag-Pro-Pol polyprotein

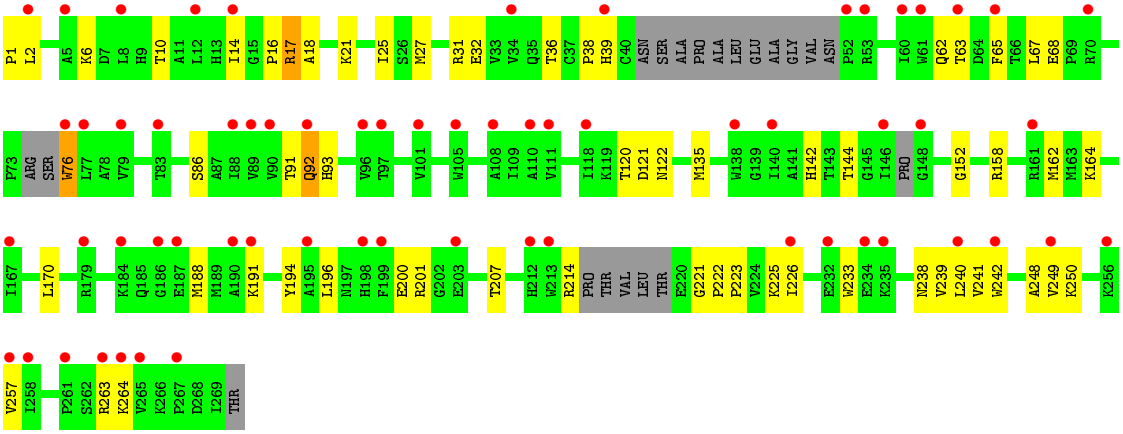
Chain C:





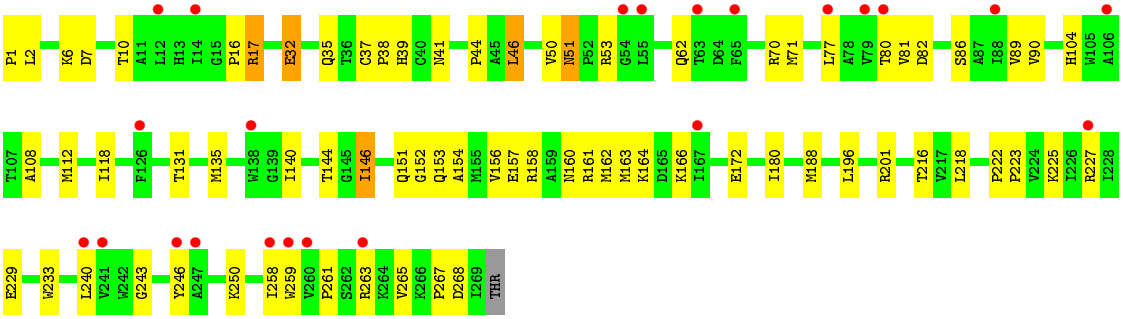
• Molecule 1: Gag-Pro-Pol polyprotein

Chain D:



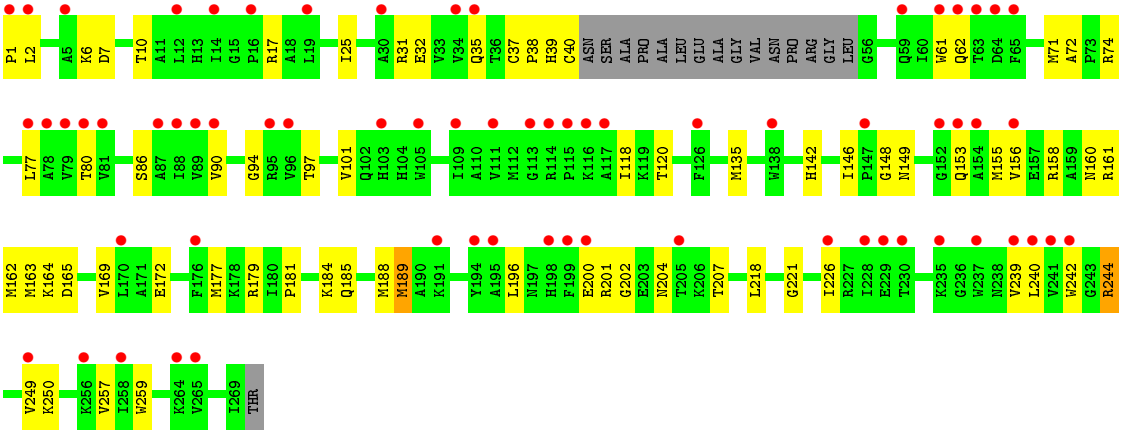
• Molecule 1: Gag-Pro-Pol polyprotein

Chain E:



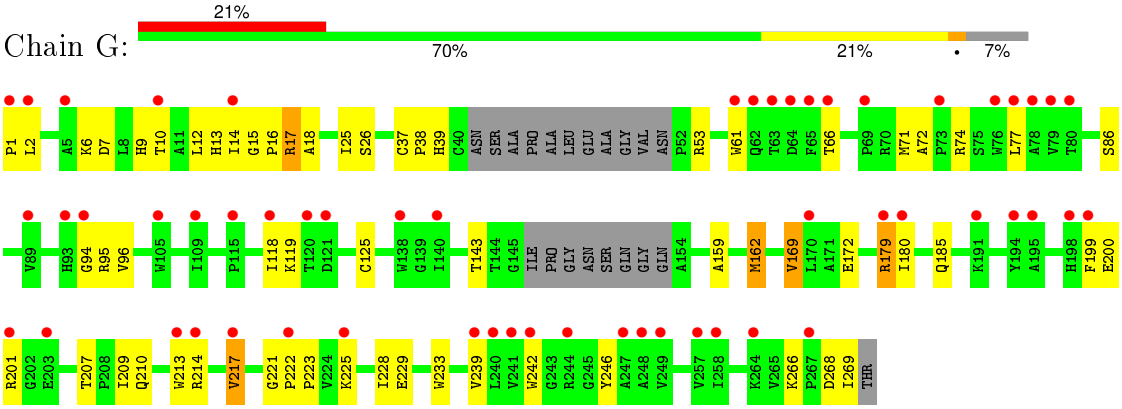
• Molecule 1: Gag-Pro-Pol polyprotein

Chain F:



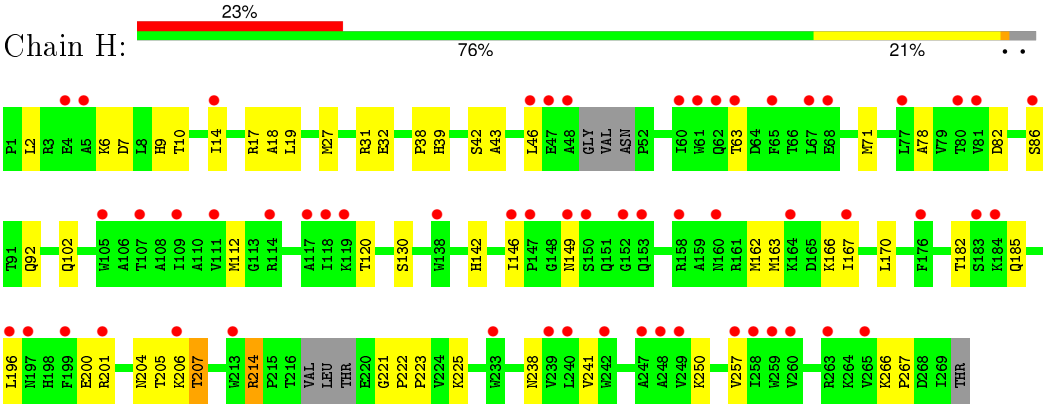
• Molecule 1: Gag-Pro-Pol polyprotein

Chain G:



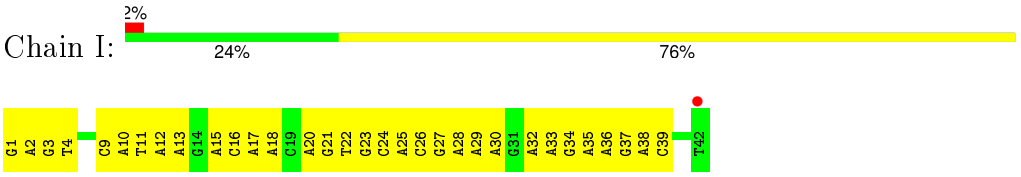
• Molecule 1: Gag-Pro-Pol polyprotein

Chain H:



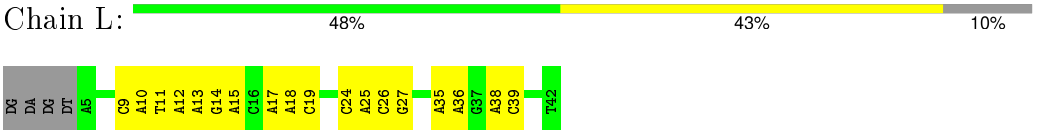
• Molecule 2: RSV Integrase

Chain I:



• Molecule 2: RSV Integrase

Chain L:

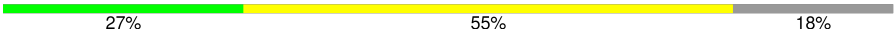


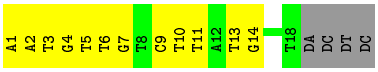
• Molecule 3: DNA (5'-D(*AP*AP*TP*GP*TP*TP*GP*TP*CP*TP*TP*AP*TP*GP*CP*AP*AP*TP*AP*CP*TP*C)-3')

Chain J:

• Molecule 3: DNA (5'-D(*AP*AP*TP*GP*TP*TP*GP*TP*CP*TP*TP*AP*TP*GP*CP*AP *AP*TP*AP*CP*TP*C)-3')

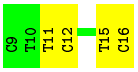
Chain M:





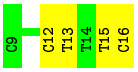
• Molecule 4: DNA (5'-D(*CP*TP*TP*CP*TP*CP*TP*C)-3')

Chain K:



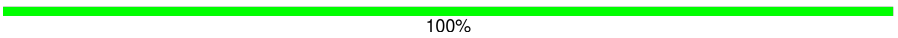
• Molecule 4: DNA (5'-D(*CP*TP*TP*CP*TP*CP*TP*C)-3')

Chain N:



• Molecule 5: DNA (5'-D(*AP*GP*TP*GP*TP*CP*TP*T)-3')

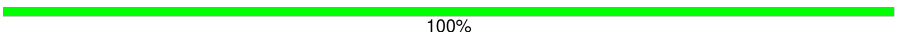
Chain k:



There are no outlier residues recorded for this chain.

• Molecule 5: DNA (5'-D(*AP*GP*TP*GP*TP*CP*TP*T)-3')

Chain n:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.94Å 157.85Å 126.58Å 90.00° 110.94° 90.00°	Depositor
Resolution (Å)	49.22 – 3.80 49.22 – 3.61	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.22-3.80) 77.5 (49.22-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 3.57Å)	Xtriage
Refinement program	PHENIX (dev_2210: ???)	Depositor
R, R_{free}	0.254 , 0.294 0.263 , 0.300	Depositor DCC
R_{free} test set	4199 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	131.0	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 150.5	EDS
Estimated twinning fraction	0.105 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 52029 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19335	wwPDB-VP
Average B, all atoms (Å^2)	206.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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

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

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	0.25	0/2139	0.47	0/2882
1	B	0.24	0/2030	0.46	0/2730
1	C	0.26	0/2046	0.51	0/2752
1	D	0.25	0/2000	0.50	0/2681
1	E	0.25	0/2139	0.48	0/2882
1	F	0.24	0/2034	0.46	0/2736
1	G	0.25	0/2008	0.47	0/2698
1	H	0.25	0/2096	0.47	0/2818
2	I	0.56	0/981	0.84	0/1513
2	L	0.53	0/888	0.84	0/1368
3	J	0.57	0/497	1.02	0/765
3	M	0.55	0/409	1.08	0/630
4	K	0.59	0/169	1.14	0/258
4	N	0.49	0/169	1.11	0/258
5	k	0.64	0/179	1.02	0/275
5	n	0.57	0/179	1.02	0/275
All	All	0.32	0/19963	0.60	0/27521

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	214	ARG	Peptide

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	2099	0	2121	49	0
1	B	1993	0	2016	30	0
1	C	2009	0	2032	55	0
1	D	1967	0	1984	46	0
1	E	2099	0	2121	64	0
1	F	1997	0	2018	45	0
1	G	1972	0	2001	43	0
1	H	2058	0	2075	38	0
2	I	869	0	470	23	0
2	L	787	0	424	16	0
3	J	445	0	253	16	0
3	M	366	0	208	12	0
4	K	154	0	95	3	0
4	N	154	0	95	2	0
5	k	161	0	94	0	0
5	n	161	0	94	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	4	0	0	0	0
7	B	20	0	0	0	0
7	F	11	0	0	0	0
7	G	1	0	0	0	0
All	All	19335	0	18101	392	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 11.

All (392) 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:H:120:THR:HG1	1:H:142:HIS:HE2	1.15	0.94
1:C:135:MSE:HE2	1:C:142:HIS:HB2	1.64	0.79
1:E:80:THR:HG1	1:E:104:HIS:HE2	1.30	0.77
2:L:12:DA:H2'	2:L:13:DA:C8	2.21	0.76
1:C:244:ARG:HH22	1:E:258:ILE:HB	1.52	0.74
1:B:39:HIS:HB3	1:B:169:VAL:HG22	1.70	0.73
1:G:17:ARG:NH1	1:G:199:PHE:O	2.21	0.73
1:C:222:PRO:HB3	1:D:257:VAL:HG11	1.69	0.73
1:F:226:ILE:HG21	1:F:249:VAL:HG21	1.69	0.73
1:B:120:THR:HG1	1:B:142:HIS:HE2	1.36	0.73
1:F:37:CYS:HB3	1:F:40:CYS:SG	2.29	0.72
1:H:86:SER:O	1:H:201:ARG:NH1	2.22	0.72
1:C:86:SER:O	1:C:201:ARG:NH1	2.24	0.70
1:F:1:PRO:HD2	1:F:2:LEU:H	1.57	0.69
1:A:27:MSE:HE3	1:A:31:ARG:HH21	1.57	0.68
1:D:1:PRO:HD2	1:D:2:LEU:H	1.59	0.68
1:G:1:PRO:HD2	1:G:2:LEU:H	1.58	0.68
1:C:1:PRO:HD2	1:C:2:LEU:H	1.59	0.67
1:E:1:PRO:HD2	1:E:2:LEU:H	1.60	0.67
1:A:38:PRO:HD2	1:A:39:HIS:H	1.60	0.67
1:E:51:ASN:ND2	1:E:152:GLY:O	2.28	0.67
1:G:72:ALA:O	1:G:179:ARG:NH1	2.29	0.66
1:E:37:CYS:O	1:E:41:ASN:ND2	2.24	0.66
1:H:71:MSE:HE2	1:H:167:ILE:HG21	1.78	0.66
1:B:1:PRO:HD2	1:B:2:LEU:H	1.59	0.66
1:H:163:MSE:HE3	1:H:167:ILE:HD11	1.77	0.66
1:D:86:SER:O	1:D:201:ARG:NH2	2.28	0.65
1:F:120:THR:OG1	1:F:142:HIS:NE2	2.27	0.65
1:E:158:ARG:HG3	3:J:5:DT:H2"	1.78	0.65
1:C:261:PRO:HD3	1:E:146:ILE:HG21	1.78	0.65
1:E:38:PRO:HD2	1:E:39:HIS:H	1.62	0.64
1:B:38:PRO:HD2	1:B:39:HIS:H	1.62	0.64
2:I:15:DA:H2'	2:I:16:DC:C6	2.32	0.64
1:E:158:ARG:NH2	3:J:6:DT:OP1	2.31	0.64
1:C:38:PRO:HD2	1:C:39:HIS:H	1.63	0.64
1:H:205:THR:HG23	1:H:206:LYS:HD2	1.79	0.64
1:F:61:TRP:HB2	1:F:118:ILE:HG12	1.80	0.64
1:E:16:PRO:HD2	1:E:17:ARG:H	1.62	0.64
1:F:90:VAL:HG11	1:F:163:MSE:HG3	1.79	0.63
2:L:13:DA:H2'	2:L:14:DG:C8	2.34	0.63
1:D:263:ARG:HH12	1:D:264:LYS:HE3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:GLY:HA3	3:J:3:DT:H5"	1.79	0.63
1:G:38:PRO:HD2	1:G:39:HIS:H	1.63	0.63
1:G:16:PRO:HD2	1:G:17:ARG:H	1.62	0.63
1:H:82:ASP:HB2	1:H:112:MSE:HE1	1.79	0.62
1:D:122:ASN:HB3	1:D:144:THR:HB	1.82	0.62
3:M:9:DC:H2'	3:M:10:DT:C6	2.34	0.62
1:E:131:THR:HG22	1:E:135:MSE:HE2	1.82	0.62
1:G:225:LYS:HE2	1:G:233:TRP:HB3	1.82	0.62
1:H:221:GLY:HA3	1:H:238:ASN:HB3	1.81	0.62
1:A:76:TRP:HB2	1:A:93:HIS:O	2.00	0.62
1:C:246:TYR:CE2	3:J:2:DA:H4'	2.35	0.62
1:F:72:ALA:HB3	1:F:179:ARG:HD2	1.81	0.62
1:H:38:PRO:HD2	1:H:39:HIS:H	1.65	0.61
1:F:86:SER:O	1:F:201:ARG:NH1	2.33	0.61
1:D:16:PRO:HD2	1:D:17:ARG:H	1.64	0.61
1:E:50:VAL:HG11	1:E:259:TRP:HB3	1.81	0.61
1:G:207:THR:OG1	1:G:210:GLN:OE1	2.18	0.61
2:I:26:DC:H2"	2:I:27:DG:H5'	1.82	0.61
1:G:223:PRO:HB2	1:G:268:ASP:HB3	1.81	0.61
1:D:221:GLY:HA3	1:D:238:ASN:HB3	1.83	0.61
1:D:38:PRO:HD2	1:D:39:HIS:H	1.65	0.61
3:J:6:DT:H2"	3:J:7:DG:C8	2.35	0.61
1:G:53:ARG:HD2	3:M:1:DA:H4'	1.83	0.60
1:F:38:PRO:HD2	1:F:39:HIS:H	1.64	0.60
1:F:135:MSE:HE2	1:F:142:HIS:HB2	1.83	0.60
1:A:144:THR:OG1	1:A:145:GLY:N	2.33	0.60
1:C:240:LEU:HD11	1:C:250:LYS:HD3	1.83	0.60
1:D:196:LEU:O	1:D:201:ARG:NE	2.31	0.60
1:C:70:ARG:NH2	1:C:177:MSE:O	2.35	0.60
1:D:240:LEU:HD11	1:D:250:LYS:HD3	1.84	0.60
1:B:227:ARG:HB3	1:B:264:LYS:HE2	1.84	0.59
1:C:61:TRP:HB2	1:C:118:ILE:HG12	1.84	0.59
3:M:1:DA:H5"	3:M:2:DA:C8	2.37	0.59
1:A:119:LYS:HG2	1:A:143:THR:HB	1.85	0.59
1:C:244:ARG:NH2	1:E:258:ILE:HB	2.18	0.59
1:A:74:ARG:HA	1:A:94:GLY:HA2	1.84	0.59
1:G:6:LYS:O	1:G:10:THR:HG23	2.03	0.59
1:G:74:ARG:HA	1:G:94:GLY:HA2	1.84	0.59
1:E:222:PRO:HB3	1:F:257:VAL:HG11	1.84	0.59
2:L:17:DA:H2'	2:L:18:DA:C8	2.38	0.59
1:C:72:ALA:O	1:C:185:GLN:NE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:PRO:HG2	1:C:264:LYS:HG3	1.86	0.58
1:F:146:ILE:HB	1:F:149:ASN:HB3	1.83	0.58
1:D:158:ARG:O	1:D:162:MSE:HB2	2.03	0.58
2:L:15:DA:H5"	2:L:15:DA:H8	1.69	0.58
1:C:27:MSE:HE3	1:C:31:ARG:HE	1.67	0.57
2:L:9:DC:O2	3:M:14:DG:N2	2.23	0.57
1:B:225:LYS:HD2	1:B:233:TRP:HB3	1.87	0.57
1:E:166:LYS:HE3	1:E:196:LEU:HD21	1.85	0.57
1:G:17:ARG:HH12	1:G:207:THR:HG22	1.70	0.57
2:I:12:DA:H2"	2:I:13:DA:H8	1.68	0.57
1:C:155:MSE:HE3	1:C:158:ARG:HH21	1.70	0.57
1:A:194:TYR:HB2	1:B:110:ALA:HA	1.86	0.57
1:G:217:VAL:HG21	1:H:214:ARG:HB3	1.87	0.57
1:G:86:SER:O	1:G:201:ARG:NH1	2.37	0.57
1:D:200:GLU:HG2	1:D:207:THR:HG22	1.85	0.56
1:A:71:MSE:HB2	1:A:75:SER:HA	1.87	0.56
1:G:39:HIS:NE2	1:G:172:GLU:OE1	2.38	0.56
1:H:27:MSE:HE3	1:H:31:ARG:HE	1.70	0.56
1:F:77:LEU:HD22	1:F:189:MSE:HE1	1.86	0.56
1:D:135:MSE:HE2	1:D:142:HIS:HB2	1.88	0.56
1:C:6:LYS:O	1:C:10:THR:HG23	2.06	0.56
1:F:6:LYS:O	1:F:10:THR:HG23	2.05	0.56
1:A:62:GLN:O	1:A:80:THR:HA	2.05	0.56
1:B:6:LYS:O	1:B:10:THR:HG23	2.06	0.56
1:C:268:ASP:OD1	1:C:269:ILE:N	2.39	0.55
1:C:246:TYR:OH	3:J:3:DT:OP1	2.20	0.55
1:A:6:LYS:O	1:A:10:THR:HG23	2.06	0.55
1:C:112:MSE:HB2	1:C:212:HIS:HE2	1.70	0.55
2:I:10:DA:H2"	2:I:11:DT:H5"	1.89	0.55
1:D:225:LYS:HD2	1:D:233:TRP:HB3	1.88	0.55
1:G:17:ARG:HH22	1:G:207:THR:HA	1.70	0.55
1:D:6:LYS:O	1:D:10:THR:HG23	2.07	0.55
1:E:6:LYS:O	1:E:10:THR:HG23	2.07	0.55
1:A:151:GLN:HE21	3:M:4:DG:H5"	1.72	0.55
1:A:204:ASN:OD1	1:A:211:LYS:NZ	2.40	0.55
1:B:68:GLU:HG3	1:B:70:ARG:H	1.72	0.55
1:G:246:TYR:OH	3:M:3:DT:OP1	2.16	0.54
1:C:112:MSE:HB2	1:C:212:HIS:NE2	2.22	0.54
1:C:246:TYR:CZ	1:E:146:ILE:HG23	2.43	0.54
1:G:179:ARG:NH1	1:G:180:ILE:O	2.40	0.54
1:H:6:LYS:O	1:H:10:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:18:DT:H2'	3:J:19:DA:C8	2.42	0.54
2:I:17:DA:H2'	2:I:18:DA:C8	2.43	0.54
1:H:46:LEU:HD13	1:H:162:MSE:HE2	1.90	0.54
1:G:61:TRP:HB2	1:G:118:ILE:HG12	1.90	0.54
1:D:239:VAL:HG11	1:D:242:TRP:HE1	1.72	0.54
1:E:71:MSE:HG3	1:E:77:LEU:HD21	1.91	0.53
1:A:146:ILE:HG12	1:A:149:ASN:HB2	1.91	0.53
1:A:156:VAL:O	1:A:159:ALA:HB3	2.08	0.53
3:J:9:DC:H2'	3:J:10:DT:C6	2.44	0.53
1:H:225:LYS:HE3	1:H:266:LYS:HB3	1.89	0.53
1:A:154:ALA:HB1	3:M:4:DG:H21	1.72	0.53
1:B:151:GLN:N	1:B:152:GLY:HA3	2.24	0.53
1:B:131:THR:HG22	1:B:135:MSE:HE2	1.91	0.53
1:G:222:PRO:HG3	1:H:257:VAL:HG11	1.91	0.52
1:F:1:PRO:O	1:F:25:ILE:HD11	2.08	0.52
1:G:1:PRO:O	1:G:25:ILE:HD11	2.10	0.52
1:A:146:ILE:HD11	1:A:149:ASN:HD22	1.74	0.52
1:C:208:PRO:HA	1:C:211:LYS:HB2	1.90	0.52
1:C:207:THR:O	1:C:211:LYS:N	2.40	0.52
1:A:81:VAL:HG12	1:A:156:VAL:HG23	1.91	0.52
2:I:25:DA:H2'	2:I:26:DC:C6	2.45	0.52
1:F:31:ARG:O	1:F:35:GLN:HG3	2.10	0.52
1:A:131:THR:HG22	1:A:135:MSE:HE2	1.91	0.52
1:D:170:LEU:HD22	1:D:191:LYS:HE3	1.91	0.52
1:E:51:ASN:ND2	1:E:62:GLN:HE22	2.08	0.51
1:C:216:THR:HG21	1:D:214:ARG:HB2	1.92	0.51
1:B:17:ARG:HE	1:B:203:GLU:HA	1.75	0.51
2:L:24:DC:H2"	2:L:25:DA:H8	1.76	0.51
1:B:7:ASP:O	1:B:10:THR:OG1	2.23	0.51
1:B:9:HIS:CE1	1:B:40:CYS:SG	3.03	0.51
1:F:239:VAL:HG11	1:F:242:TRP:HE1	1.75	0.51
1:C:246:TYR:HH	1:E:146:ILE:HG12	1.76	0.51
1:E:146:ILE:HD11	3:J:3:DT:H5'	1.93	0.51
1:C:114:ARG:NH1	1:D:194:TYR:OH	2.44	0.51
1:C:267:PRO:HD2	1:E:44:PRO:HB2	1.92	0.51
2:I:12:DA:H4'	2:I:13:DA:OP1	2.10	0.51
1:C:266:LYS:HD2	1:E:44:PRO:HD2	1.93	0.51
1:E:153:GLN:O	1:E:156:VAL:HG12	2.11	0.51
1:C:225:LYS:HD3	1:C:266:LYS:HZ2	1.76	0.51
2:I:32:DA:H2"	2:I:33:DA:C8	2.46	0.51
1:A:225:LYS:HE2	1:A:233:TRP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:HIS:CG	1:C:213:TRP:H	2.27	0.51
1:F:17:ARG:HH11	1:F:202:GLY:HA2	1.77	0.50
4:K:15:DT:H2'	4:K:16:DC:C6	2.46	0.50
1:E:267:PRO:HB3	1:F:259:TRP:CD2	2.47	0.50
2:L:11:DT:H2'	2:L:12:DA:C8	2.46	0.50
1:A:78:ALA:O	1:A:90:VAL:HA	2.11	0.50
1:A:151:GLN:HB2	3:M:4:DG:OP2	2.10	0.50
1:E:164:LYS:NZ	2:I:20:DA:OP1	2.44	0.50
1:E:35:GLN:O	1:E:41:ASN:ND2	2.45	0.49
1:A:172:GLU:HB3	1:E:39:HIS:CE1	2.46	0.49
1:D:241:VAL:HB	1:D:248:ALA:HB3	1.94	0.49
1:A:42:SER:N	1:A:43:ALA:HA	2.28	0.49
1:B:60:ILE:HD13	1:B:119:LYS:HE3	1.95	0.49
1:H:92:GLN:HB3	1:H:189:MSE:HE1	1.93	0.49
2:L:38:DA:H2"	2:L:39:DC:C5	2.48	0.49
1:F:74:ARG:HA	1:F:94:GLY:HA2	1.94	0.49
1:D:263:ARG:CZ	1:E:32:GLU:HB2	2.42	0.49
1:C:216:THR:HG21	1:D:214:ARG:HD2	1.94	0.49
1:G:242:TRP:CZ3	1:H:241:VAL:HG11	2.48	0.49
1:C:12:LEU:HB2	1:C:14:ILE:HG13	1.95	0.49
1:F:72:ALA:O	1:F:185:GLN:NE2	2.45	0.49
1:C:14:ILE:CG2	1:C:18:ALA:HB3	2.43	0.49
1:D:222:PRO:HB2	1:D:223:PRO:O	2.12	0.49
4:K:11:DT:H2"	4:K:12:DC:O5'	2.11	0.49
1:H:42:SER:N	1:H:43:ALA:HA	2.27	0.49
1:D:76:TRP:N	1:D:93:HIS:O	2.46	0.49
2:I:33:DA:H2"	2:I:34:DG:C8	2.47	0.49
1:E:225:LYS:HE2	1:E:233:TRP:HB3	1.95	0.48
1:D:239:VAL:HG21	1:D:242:TRP:NE1	2.28	0.48
1:H:222:PRO:HB2	1:H:223:PRO:O	2.12	0.48
1:A:42:SER:HB2	1:A:43:ALA:C	2.34	0.48
1:E:157:GLU:OE1	1:E:160:ASN:ND2	2.46	0.48
1:H:17:ARG:NE	1:H:204:ASN:H	2.12	0.48
1:H:146:ILE:O	1:H:149:ASN:ND2	2.46	0.48
3:M:4:DG:H4'	3:M:5:DT:OP1	2.14	0.48
1:B:239:VAL:HG11	1:B:242:TRP:CZ2	2.48	0.48
2:I:28:DA:H2"	2:I:29:DA:H8	1.78	0.48
4:N:12:DC:H2"	4:N:13:DT:H5"	1.94	0.48
1:H:200:GLU:HG3	1:H:207:THR:HB	1.95	0.48
1:G:66:THR:HG23	1:G:77:LEU:HB2	1.96	0.48
2:I:1:DG:H2"	2:I:2:DA:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:SER:O	1:E:201:ARG:NH2	2.46	0.48
1:E:7:ASP:O	1:E:10:THR:OG1	2.27	0.48
1:A:146:ILE:HD12	1:A:147:PRO:HD2	1.95	0.48
1:A:61:TRP:HB2	1:A:118:ILE:HG12	1.95	0.48
2:I:29:DA:H2"	2:I:30:DA:C8	2.49	0.48
1:G:71:MSE:HE1	1:G:185:GLN:HB3	1.95	0.48
3:J:7:DG:H2"	3:J:8:DT:H5"	1.96	0.47
1:A:43:ALA:HB3	1:G:266:LYS:HB2	1.96	0.47
1:G:9:HIS:HE2	1:G:37:CYS:CB	2.21	0.47
2:L:18:DA:H2"	2:L:19:DC:C5	2.48	0.47
1:G:96:VAL:HG12	1:G:125:CYS:SG	2.55	0.47
1:C:200:GLU:HG3	1:C:207:THR:HA	1.96	0.47
1:D:122:ASN:N	1:D:122:ASN:OD1	2.48	0.47
1:B:21:LYS:NZ	1:B:205:THR:O	2.47	0.47
1:C:2:LEU:O	1:C:6:LYS:HG3	2.14	0.47
1:F:240:LEU:HD11	1:F:250:LYS:HD3	1.97	0.47
1:C:17:ARG:CZ	1:C:200:GLU:HB3	2.44	0.47
1:H:2:LEU:O	1:H:6:LYS:HG3	2.14	0.47
1:F:158:ARG:O	1:F:162:MSE:HG2	2.15	0.47
1:C:214:ARG:HB2	1:C:217:VAL:HG22	1.97	0.47
3:J:13:DT:H2"	3:J:14:DG:H5'	1.97	0.47
2:I:36:DA:H2"	2:I:37:DG:C8	2.49	0.46
1:A:248:ALA:HB2	1:A:259:TRP:CZ3	2.50	0.46
1:E:82:ASP:HB2	1:E:112:MSE:HE1	1.97	0.46
1:A:39:HIS:ND1	1:E:172:GLU:HB3	2.30	0.46
1:C:250:LYS:HD2	1:C:255:ASP:OD1	2.14	0.46
1:C:89:VAL:HG23	1:C:112:MSE:HE3	1.97	0.46
1:C:21:LYS:NZ	1:C:205:THR:O	2.48	0.46
1:E:216:THR:HA	1:F:218:LEU:HB2	1.96	0.46
3:M:6:DT:H2"	3:M:7:DG:C8	2.50	0.46
1:A:63:THR:HA	1:A:79:VAL:O	2.15	0.46
1:H:90:VAL:HG11	1:H:163:MSE:HE2	1.97	0.46
1:F:162:MSE:HE2	1:F:201:ARG:HH21	1.81	0.46
1:E:81:VAL:HG12	1:E:156:VAL:HG23	1.98	0.46
4:K:11:DT:H2'	4:K:12:DC:C6	2.51	0.46
1:A:51:ASN:ND2	1:A:246:TYR:HB3	2.30	0.46
1:D:263:ARG:NH1	1:E:32:GLU:HB2	2.31	0.45
3:M:10:DT:H2'	3:M:11:DT:C6	2.51	0.45
2:I:34:DG:H2"	2:I:35:DA:C8	2.51	0.45
1:F:162:MSE:HB3	1:F:196:LEU:HD21	1.97	0.45
2:L:9:DC:H2'	2:L:10:DA:C5	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:GLU:O	1:D:36:THR:HG23	2.15	0.45
1:H:266:LYS:HG2	1:H:267:PRO:HD2	1.98	0.45
1:E:223:PRO:HB2	1:E:268:ASP:HB3	1.98	0.45
1:B:90:VAL:HG13	1:B:189:MSE:HE3	1.98	0.45
3:M:13:DT:H2"	3:M:14:DG:C8	2.52	0.45
1:F:62:GLN:OE1	1:F:155:MSE:HB3	2.17	0.45
2:I:3:DG:H2'	2:I:4:DT:H71	1.99	0.45
1:F:7:ASP:O	1:F:10:THR:OG1	2.23	0.45
1:F:200:GLU:HG3	1:F:207:THR:HG22	1.99	0.45
1:H:63:THR:HB	1:H:120:THR:HG22	1.98	0.45
1:F:39:HIS:HB3	1:F:169:VAL:HG22	1.99	0.45
1:A:17:ARG:HA	1:A:17:ARG:HD2	1.43	0.45
3:J:20:DC:H2'	3:J:21:DT:C6	2.52	0.45
1:D:62:GLN:HE22	1:D:152:GLY:HA3	1.80	0.45
1:H:170:LEU:HB2	1:H:188:MSE:HE1	1.99	0.45
1:E:2:LEU:O	1:E:6:LYS:HG3	2.17	0.44
1:E:50:VAL:HG22	1:E:246:TYR:CE2	2.52	0.44
1:H:7:ASP:O	1:H:10:THR:OG1	2.24	0.44
2:I:38:DA:H2"	2:I:39:DC:C6	2.53	0.44
1:D:67:LEU:HB2	1:D:76:TRP:CZ2	2.52	0.44
1:A:164:LYS:O	1:A:167:ILE:HB	2.16	0.44
1:F:2:LEU:O	1:F:6:LYS:HG3	2.17	0.44
1:B:2:LEU:O	1:B:6:LYS:HG3	2.18	0.44
1:F:181:PRO:O	1:F:185:GLN:HG3	2.17	0.44
1:E:246:TYR:CD2	1:E:261:PRO:HA	2.52	0.44
1:F:239:VAL:HG21	1:F:242:TRP:NE1	2.33	0.44
1:E:240:LEU:HD11	1:E:250:LYS:HD3	2.00	0.44
1:E:90:VAL:HG21	1:E:163:MSE:HE2	1.98	0.44
1:F:160:ASN:HB3	1:F:164:LYS:HE2	1.99	0.44
1:B:70:ARG:HH21	1:B:178:LYS:HA	1.83	0.44
3:J:18:DT:H2"	3:J:19:DA:O5'	2.17	0.44
1:G:7:ASP:O	1:G:10:THR:OG1	2.28	0.44
1:F:148:GLY:HA2	1:F:153:GLN:HG3	1.98	0.44
1:C:71:MSE:HE2	1:C:189:MSE:HE3	1.99	0.44
1:D:27:MSE:HE3	1:D:31:ARG:HE	1.82	0.44
1:A:228:ILE:HG13	1:A:229:GLU:N	2.33	0.44
2:L:17:DA:H2"	2:L:18:DA:O5'	2.18	0.44
2:L:15:DA:H5"	2:L:15:DA:C8	2.49	0.44
1:H:166:LYS:HE3	1:H:196:LEU:HD21	1.99	0.43
2:L:26:DC:H2"	2:L:27:DG:H5'	1.99	0.43
1:E:80:THR:OG1	1:E:104:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:12:DA:H2'	2:L:13:DA:H8	1.76	0.43
1:F:184:LYS:O	1:F:188:MSE:HG2	2.18	0.43
1:C:61:TRP:CE3	1:C:115:PRO:HG3	2.53	0.43
1:C:82:ASP:HB3	1:C:85:SER:HB2	2.00	0.43
1:G:14:ILE:CG2	1:G:18:ALA:HB3	2.48	0.43
1:A:2:LEU:O	1:A:6:LYS:HG3	2.18	0.43
1:E:218:LEU:HD21	1:F:240:LEU:HB3	2.01	0.43
1:B:90:VAL:HG11	1:B:163:MSE:HE2	2.00	0.43
1:B:80:THR:OG1	1:B:104:HIS:NE2	2.33	0.43
1:G:268:ASP:O	1:G:269:ILE:HB	2.19	0.43
1:G:159:ALA:HA	1:G:162:MSE:HB2	1.99	0.43
2:I:9:DC:H2"	2:I:10:DA:OP2	2.18	0.43
4:N:15:DT:H2"	4:N:16:DC:C6	2.53	0.43
1:D:226:ILE:HG21	1:D:249:VAL:HG21	2.01	0.43
1:H:9:HIS:HB2	1:H:19:LEU:HD11	2.01	0.43
1:G:25:ILE:HG22	1:G:26:SER:O	2.18	0.43
1:E:162:MSE:HE2	1:E:196:LEU:HD22	2.01	0.43
1:H:162:MSE:HE3	1:H:162:MSE:HB3	1.93	0.43
1:H:250:LYS:HB2	1:H:257:VAL:HG22	2.00	0.43
1:C:225:LYS:HE2	1:C:233:TRP:HB3	2.01	0.43
1:G:242:TRP:CE3	1:H:241:VAL:HG21	2.54	0.43
1:G:15:GLY:HA3	1:G:200:GLU:OE2	2.19	0.43
2:I:11:DT:H2"	2:I:12:DA:H8	1.83	0.43
1:D:14:ILE:CG2	1:D:18:ALA:HB3	2.49	0.43
1:E:151:GLN:O	1:E:154:ALA:HB2	2.19	0.43
1:D:263:ARG:NH1	1:D:264:LYS:HE3	2.32	0.43
1:A:32:GLU:O	1:A:36:THR:HG23	2.19	0.43
1:F:221:GLY:HA3	1:F:239:VAL:O	2.19	0.42
1:C:222:PRO:HB3	1:D:257:VAL:CG1	2.46	0.42
1:H:78:ALA:O	1:H:90:VAL:HA	2.19	0.42
1:C:77:LEU:HD22	1:C:189:MSE:HE1	2.01	0.42
1:H:14:ILE:CG2	1:H:18:ALA:HB3	2.50	0.42
1:G:228:ILE:HG13	1:G:229:GLU:N	2.34	0.42
1:A:239:VAL:HG13	1:B:241:VAL:HG21	2.00	0.42
1:B:239:VAL:HG21	1:B:242:TRP:CE2	2.54	0.42
1:F:62:GLN:O	1:F:80:THR:HA	2.19	0.42
1:E:227:ARG:NH2	1:E:263:ARG:HH12	2.17	0.42
2:L:11:DT:H2'	2:L:12:DA:H8	1.82	0.42
1:A:226:ILE:HA	1:A:264:LYS:O	2.19	0.42
3:J:16:DA:H2"	3:J:17:DA:C8	2.55	0.42
1:G:119:LYS:HG2	1:G:143:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:THR:HG22	1:B:144:THR:HG21	2.01	0.42
1:E:53:ARG:HH12	1:E:243:GLY:HA3	1.85	0.42
1:G:12:LEU:HB2	1:G:14:ILE:HG13	2.01	0.42
1:G:209:ILE:HG23	1:G:213:TRP:HD1	1.84	0.42
1:E:158:ARG:HG2	1:E:161:ARG:CZ	2.49	0.42
1:A:159:ALA:O	1:A:163:MSE:N	2.52	0.42
1:E:188:MSE:HE3	1:E:188:MSE:HB3	1.92	0.42
1:A:246:TYR:CD1	1:A:261:PRO:HA	2.54	0.42
1:A:48:ALA:HB3	1:A:263:ARG:HH21	1.85	0.42
1:A:38:PRO:CB	1:G:269:ILE:HG12	2.49	0.42
1:C:158:ARG:HG2	1:C:161:ARG:NH1	2.34	0.42
2:L:35:DA:H2"	2:L:36:DA:C8	2.54	0.42
1:C:265:VAL:O	1:E:46:LEU:HB3	2.20	0.42
1:G:221:GLY:HA3	1:G:239:VAL:O	2.20	0.42
1:C:246:TYR:OH	1:E:146:ILE:HG12	2.20	0.42
1:G:217:VAL:CG2	1:H:214:ARG:HB3	2.49	0.42
1:A:153:GLN:O	1:A:156:VAL:HG12	2.20	0.42
1:E:70:ARG:HB3	1:E:180:ILE:HG13	2.02	0.42
2:I:21:DG:H3'	2:I:22:DT:H71	2.02	0.41
1:C:65:PHE:HE2	1:C:101:VAL:HG22	1.85	0.41
1:C:246:TYR:HH	3:J:3:DT:P	2.41	0.41
1:E:53:ARG:HB2	1:E:259:TRP:CH2	2.55	0.41
2:I:11:DT:H2"	2:I:12:DA:C8	2.54	0.41
1:G:13:HIS:ND1	1:G:37:CYS:SG	2.91	0.41
1:C:151:GLN:HG3	1:C:152:GLY:H	1.85	0.41
2:I:23:DG:H2"	2:I:24:DC:C6	2.55	0.41
1:D:92:GLN:HE21	1:D:92:GLN:HB3	1.57	0.41
1:F:1:PRO:HD2	1:F:2:LEU:N	2.32	0.41
2:I:35:DA:H2"	2:I:36:DA:C8	2.56	0.41
1:D:188:MSE:HE2	1:D:188:MSE:HB3	1.97	0.41
1:D:67:LEU:HD23	1:D:76:TRP:HA	2.03	0.41
1:F:97:THR:O	1:F:101:VAL:HG23	2.20	0.41
1:C:17:ARG:HH21	1:C:201:ARG:C	2.24	0.41
1:H:223:PRO:HB3	1:H:238:ASN:ND2	2.35	0.41
1:F:71:MSE:HE1	1:F:185:GLN:HB3	2.03	0.41
1:B:221:GLY:HA3	1:B:239:VAL:O	2.21	0.41
1:D:63:THR:HB	1:D:120:THR:HG22	2.03	0.41
1:D:68:GLU:HB2	1:D:164:LYS:HG2	2.03	0.41
1:C:12:LEU:HD12	1:C:14:ILE:HD11	2.01	0.41
1:B:241:VAL:HB	1:B:248:ALA:HB3	2.03	0.41
1:E:118:ILE:HG13	1:E:140:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:VAL:O	1:F:244:ARG:NH1	2.53	0.41
1:F:161:ARG:O	1:F:165:ASP:HB2	2.21	0.41
1:D:1:PRO:O	1:D:25:ILE:HD11	2.20	0.41
1:E:144:THR:O	3:J:2:DA:H5"	2.21	0.41
1:B:1:PRO:HD2	1:B:2:LEU:N	2.33	0.41
1:A:203:GLU:HB3	1:E:17:ARG:HH11	1.84	0.41
1:D:242:TRP:HB2	1:E:229:GLU:HG2	2.02	0.41
1:A:246:TYR:HD1	1:A:261:PRO:HA	1.85	0.41
1:B:61:TRP:HB2	1:B:118:ILE:HG12	2.01	0.41
1:H:102:GLN:NE2	1:H:130:SER:OG	2.50	0.41
1:F:172:GLU:HG2	1:F:177:MSE:SE	2.71	0.41
1:D:65:PHE:HB3	1:D:76:TRP:CZ3	2.56	0.41
1:G:13:HIS:CD2	1:G:169:VAL:HG13	2.56	0.41
1:A:248:ALA:HB2	1:A:259:TRP:CH2	2.56	0.41
1:B:61:TRP:CE3	1:B:115:PRO:HG3	2.55	0.41
1:H:182:THR:HA	1:H:185:GLN:HG3	2.02	0.41
1:D:1:PRO:HD2	1:D:2:LEU:N	2.33	0.40
1:A:172:GLU:HB3	1:E:39:HIS:ND1	2.36	0.40
1:A:48:ALA:O	1:A:50:VAL:HG22	2.20	0.40
1:E:89:VAL:HG11	1:E:108:ALA:HA	2.03	0.40
1:A:122:ASN:HB3	1:A:144:THR:OG1	2.21	0.40
1:D:121:ASP:OD1	1:D:121:ASP:N	2.55	0.40
1:D:17:ARG:HD3	1:D:21:LYS:HE3	2.03	0.40

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	267/270 (99%)	253 (95%)	14 (5%)	0	100	100
1	B	249/270 (92%)	243 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	252/270 (93%)	237 (94%)	13 (5%)	2 (1%)	24 70
1	D	240/270 (89%)	230 (96%)	10 (4%)	0	100 100
1	E	267/270 (99%)	254 (95%)	13 (5%)	0	100 100
1	F	250/270 (93%)	244 (98%)	6 (2%)	0	100 100
1	G	244/270 (90%)	236 (97%)	8 (3%)	0	100 100
1	H	257/270 (95%)	248 (96%)	9 (4%)	0	100 100
All	All	2026/2160 (94%)	1945 (96%)	79 (4%)	2 (0%)	56 90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	213	TRP
1	C	212	HIS

5.3.2 Protein sidechains (i)

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	222/212 (105%)	213 (96%)	9 (4%)	37 74
1	B	212/212 (100%)	212 (100%)	0	100 100
1	C	213/212 (100%)	208 (98%)	5 (2%)	58 84
1	D	207/212 (98%)	203 (98%)	4 (2%)	65 87
1	E	222/212 (105%)	217 (98%)	5 (2%)	58 84
1	F	212/212 (100%)	207 (98%)	5 (2%)	57 84
1	G	209/212 (99%)	203 (97%)	6 (3%)	50 81
1	H	217/212 (102%)	214 (99%)	3 (1%)	74 90
All	All	1714/1696 (101%)	1677 (98%)	37 (2%)	60 85

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	46	LEU
1	A	53	ARG
1	A	144	THR
1	A	146	ILE
1	A	153	GLN
1	A	156	VAL
1	A	165	ASP
1	A	266	LYS
1	C	155	MSE
1	C	207	THR
1	C	213	TRP
1	C	218	LEU
1	C	220	GLU
1	D	17	ARG
1	D	76	TRP
1	D	91	THR
1	D	92	GLN
1	E	17	ARG
1	E	32	GLU
1	E	46	LEU
1	E	51	ASN
1	E	146	ILE
1	F	32	GLU
1	F	156	VAL
1	F	189	MSE
1	F	204	ASN
1	F	244	ARG
1	G	17	ARG
1	G	95	ARG
1	G	162	MSE
1	G	169	VAL
1	G	179	ARG
1	G	217	VAL
1	H	32	GLU
1	H	207	THR
1	H	214	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	B	102	GLN

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Mol	Chain	Res	Type
1	B	153	GLN
1	D	92	GLN
1	D	142	HIS
1	E	51	ASN
1	E	151	GLN
1	F	102	GLN
1	H	102	GLN
1	H	153	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 44 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

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	258/270 (95%)	0.93	47 (18%) 2 1	140, 172, 220, 265	0
1	B	242/270 (89%)	0.92	42 (17%) 2 2	151, 195, 256, 283	0
1	C	245/270 (90%)	0.88	37 (15%) 3 2	152, 191, 249, 263	0
1	D	239/270 (88%)	1.19	63 (26%) 1 1	177, 201, 248, 277	0
1	E	258/270 (95%)	0.70	23 (8%) 12 7	140, 177, 210, 220	0
1	F	243/270 (90%)	1.34	67 (27%) 1 1	185, 210, 250, 265	0
1	G	239/270 (88%)	1.07	56 (23%) 1 1	158, 201, 282, 302	0
1	H	252/270 (93%)	1.14	63 (25%) 1 1	173, 198, 230, 242	0
2	I	42/42 (100%)	-0.11	1 (2%) 62 46	173, 261, 354, 378	0
2	L	38/42 (90%)	-0.10	0 100 100	176, 221, 315, 333	0
3	J	22/22 (100%)	-0.17	0 100 100	158, 275, 316, 334	0
3	M	18/22 (81%)	-0.10	0 100 100	175, 216, 329, 333	0
4	K	8/8 (100%)	-0.07	0 100 100	174, 210, 275, 299	0
4	N	8/8 (100%)	-0.13	0 100 100	171, 192, 252, 269	0
5	k	8/8 (100%)	-0.35	0 100 100	347, 360, 364, 366	0
5	n	8/8 (100%)	-0.46	0 100 100	279, 301, 333, 334	0
All	All	2128/2320 (91%)	0.94	399 (18%) 2 1	140, 197, 265, 378	0

All (399) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	153	GLN	15.2
1	F	114	ARG	14.2
1	D	52	PRO	10.0
1	H	146	ILE	9.3
1	F	63	THR	8.9

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Mol	Chain	Res	Type	RSRZ
1	F	113	GLY	8.5
1	B	153	GLN	7.8
1	C	147	PRO	7.3
1	H	118	ILE	7.0
1	D	187	GLU	6.9
1	H	88	ILE	6.8
1	D	88	ILE	6.8
1	G	2	LEU	6.4
1	F	88	ILE	6.3
1	F	115	PRO	6.2
1	F	64	ASP	6.2
1	G	64	ASP	6.2
1	E	55	LEU	6.0
1	G	94	GLY	6.0
1	B	249	VAL	6.0
1	G	63	THR	6.0
1	F	105	TRP	5.8
1	A	218	LEU	5.6
1	C	14	ILE	5.5
1	A	105	TRP	5.3
1	A	242	TRP	5.3
1	H	138	TRP	5.3
1	A	233	TRP	5.3
1	G	65	PHE	5.3
1	B	67	LEU	5.2
1	F	16	PRO	5.2
1	D	96	VAL	5.2
1	A	63	THR	5.1
1	F	147	PRO	5.1
1	F	62	GLN	5.0
1	E	247	ALA	5.0
1	G	199	PHE	5.0
1	G	105	TRP	5.0
1	B	206	LYS	5.0
1	H	114	ARG	4.9
1	B	65	PHE	4.9
1	F	199	PHE	4.9
1	B	63	THR	4.9
1	B	76	TRP	4.9
1	D	92	GLN	4.9
1	H	5	ALA	4.9
1	A	240	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	61	TRP	4.7
1	F	65	PHE	4.7
1	H	259	TRP	4.7
1	A	257	VAL	4.7
1	G	191	LYS	4.7
1	H	63	THR	4.7
1	A	239	VAL	4.7
1	F	240	LEU	4.7
1	E	138	TRP	4.6
1	C	198	HIS	4.6
1	F	80	THR	4.6
1	F	229	GLU	4.6
1	E	240	LEU	4.5
1	F	230	THR	4.5
1	G	240	LEU	4.5
1	G	1	PRO	4.5
1	H	61	TRP	4.4
1	A	49	GLY	4.4
1	B	77	LEU	4.4
1	F	200	GLU	4.4
1	H	87	ALA	4.4
1	H	258	ILE	4.4
1	B	152	GLY	4.4
1	D	186	GLY	4.4
1	C	191	LYS	4.3
1	B	62	GLN	4.3
1	E	14	ILE	4.3
1	F	239	VAL	4.3
1	D	249	VAL	4.3
1	B	179	ARG	4.2
1	C	242	TRP	4.2
1	C	95	ARG	4.2
1	D	240	LEU	4.2
1	D	138	TRP	4.2
1	D	199	PHE	4.2
1	D	89	VAL	4.2
1	B	64	ASP	4.1
1	D	148	GLY	4.1
1	C	216	THR	4.1
1	D	39	HIS	4.0
1	D	191	LYS	4.0
1	F	95	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	147	PRO	4.0
1	F	228	ILE	3.9
1	A	249	VAL	3.9
1	D	232	GLU	3.9
1	F	264	LYS	3.9
1	F	34	VAL	3.9
1	F	89	VAL	3.8
1	E	63	THR	3.8
1	H	184	LYS	3.8
1	C	146	ILE	3.8
1	G	258	ILE	3.8
1	H	149	ASN	3.8
1	G	76	TRP	3.8
1	G	217	VAL	3.7
1	G	242	TRP	3.7
1	B	61	TRP	3.7
1	H	119	LYS	3.6
1	A	2	LEU	3.6
1	E	88	ILE	3.6
1	F	79	VAL	3.6
1	H	89	VAL	3.6
1	B	105	TRP	3.6
1	G	198	HIS	3.6
1	D	90	VAL	3.6
1	F	242	TRP	3.6
1	H	47	GLU	3.6
1	H	206	LYS	3.6
1	F	77	LEU	3.6
1	G	222	PRO	3.5
1	B	2	LEU	3.5
1	B	259	TRP	3.5
1	F	154	ALA	3.5
1	H	46	LEU	3.5
1	C	194	TYR	3.4
1	G	194	TYR	3.4
1	A	265	VAL	3.4
1	B	244	ARG	3.4
1	D	213	TRP	3.4
1	G	118	ILE	3.4
1	H	117	ALA	3.4
1	B	180	ILE	3.4
1	H	183	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	73	PRO	3.3
1	G	195	ALA	3.3
1	G	239	VAL	3.3
1	D	34	VAL	3.3
1	F	138	TRP	3.3
1	D	60	ILE	3.3
1	F	226	ILE	3.3
1	F	241	VAL	3.3
1	H	67	LEU	3.3
1	D	212	HIS	3.3
1	H	248	ALA	3.3
1	C	105	TRP	3.2
1	B	147	PRO	3.2
1	A	119	LYS	3.2
1	G	93	HIS	3.2
1	H	4	GLU	3.2
1	H	213	TRP	3.2
1	D	118	ILE	3.2
1	H	14	ILE	3.2
1	C	115	PRO	3.2
1	G	14	ILE	3.2
1	C	119	LYS	3.2
1	A	12	LEU	3.2
1	G	69	PRO	3.2
1	D	97	THR	3.2
1	G	109	ILE	3.2
1	D	2	LEU	3.2
1	G	213	TRP	3.1
1	E	258	ILE	3.1
1	C	145	GLY	3.1
1	C	199	PHE	3.1
1	G	61	TRP	3.1
1	F	194	TYR	3.1
1	D	110	ALA	3.1
1	D	77	LEU	3.1
1	C	180	ILE	3.1
1	F	258	ILE	3.1
1	D	184	LYS	3.0
1	E	12	LEU	3.0
1	B	240	LEU	3.0
1	F	1	PRO	3.0
1	F	96	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	249	VAL	3.0
1	D	242	TRP	3.0
1	B	201	ARG	3.0
1	G	121	ASP	3.0
1	F	191	LYS	3.0
1	D	179	ARG	3.0
1	F	59	GLN	3.0
1	D	161	ARG	3.0
1	A	258	ILE	3.0
1	A	65	PHE	3.0
1	H	80	THR	3.0
1	H	247	ALA	3.0
1	C	267	PRO	3.0
1	H	164	LYS	3.0
2	I	42	DT	3.0
1	B	68	GLU	2.9
1	H	60	ILE	2.9
1	H	62	GLN	2.9
1	D	83	THR	2.9
1	D	111	VAL	2.9
1	E	260	VAL	2.9
1	H	199	PHE	2.9
1	H	167	ILE	2.9
1	B	72	ALA	2.9
1	H	48	ALA	2.9
1	E	65	PHE	2.9
1	D	234	GLU	2.9
1	D	65	PHE	2.9
1	G	267	PRO	2.9
1	D	8	LEU	2.9
1	G	179	ARG	2.9
1	D	12	LEU	2.8
1	A	14	ILE	2.8
1	D	79	VAL	2.8
1	A	255	ASP	2.8
1	C	109	ILE	2.8
1	H	68	GLU	2.8
1	D	101	VAL	2.8
1	B	269	ILE	2.8
1	G	241	VAL	2.8
1	B	267	PRO	2.8
1	G	5	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	201	ARG	2.8
1	A	48	ALA	2.8
1	A	256	LYS	2.8
1	H	242	TRP	2.7
1	F	111	VAL	2.7
1	H	77	LEU	2.7
1	F	103	HIS	2.7
1	B	60	ILE	2.7
1	H	196	LEU	2.7
1	E	259	TRP	2.7
1	A	221	GLY	2.7
1	C	60	ILE	2.7
1	D	76	TRP	2.7
1	B	12	LEU	2.7
1	F	109	ILE	2.7
1	B	66	THR	2.7
1	F	256	LYS	2.7
1	F	81	VAL	2.7
1	B	118	ILE	2.7
1	D	203	GLU	2.7
1	F	12	LEU	2.7
1	H	65	PHE	2.7
1	H	81	VAL	2.7
1	G	257	VAL	2.6
1	A	262	SER	2.6
1	H	150	SER	2.6
1	D	235	LYS	2.6
1	G	80	THR	2.6
1	F	156	VAL	2.6
1	G	180	ILE	2.6
1	F	5	ALA	2.6
1	B	119	LYS	2.6
1	E	79	VAL	2.6
1	E	77	LEU	2.6
1	A	88	ILE	2.6
1	C	257	VAL	2.6
1	F	235	LYS	2.6
1	D	14	ILE	2.6
1	E	263	ARG	2.6
1	B	88	ILE	2.6
1	F	198	HIS	2.6
1	B	1	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	240	LEU	2.6
1	G	203	GLU	2.6
1	F	116	LYS	2.6
1	H	160	ASN	2.6
1	H	195	ALA	2.6
1	C	90	VAL	2.6
1	F	265	VAL	2.6
1	H	239	VAL	2.6
1	H	257	VAL	2.6
1	A	5	ALA	2.6
1	F	176	PHE	2.6
1	H	249	VAL	2.5
1	D	70	ARG	2.5
1	A	77	LEU	2.5
1	B	213	TRP	2.5
1	D	267	PRO	2.5
1	A	81	VAL	2.5
1	G	62	GLN	2.5
1	A	149	ASN	2.5
1	D	261	PRO	2.5
1	A	45	ALA	2.5
1	D	190	ALA	2.5
1	G	140	ILE	2.5
1	A	176	PHE	2.5
1	G	248	ALA	2.4
1	G	77	LEU	2.4
1	D	53	ARG	2.4
1	D	258	ILE	2.4
1	D	264	LYS	2.4
1	E	54	GLY	2.4
1	A	31	ARG	2.4
1	C	187	GLU	2.4
1	C	176	PHE	2.4
1	G	138	TRP	2.4
1	A	222	PRO	2.4
1	A	191	LYS	2.4
1	F	170	LEU	2.4
1	H	233	TRP	2.4
1	F	87	ALA	2.4
1	A	138	TRP	2.4
1	F	14	ILE	2.4
1	D	63	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	114	ARG	2.4
1	C	114	ARG	2.4
1	F	19	LEU	2.4
1	A	47	GLU	2.4
1	G	214	ARG	2.4
1	C	67	LEU	2.4
1	C	247	ALA	2.4
1	D	257	VAL	2.4
1	F	152	GLY	2.4
1	B	192	ALA	2.4
1	C	209	ILE	2.3
1	D	61	TRP	2.3
1	A	170	LEU	2.3
1	A	247	ALA	2.3
1	F	90	VAL	2.3
1	G	89	VAL	2.3
1	C	167	ILE	2.3
1	E	80	THR	2.3
1	F	35	GLN	2.3
1	H	111	VAL	2.3
1	D	263	ARG	2.3
1	E	241	VAL	2.3
1	G	66	THR	2.3
1	H	153	GLN	2.3
1	D	167	ILE	2.3
1	H	109	ILE	2.3
1	A	67	LEU	2.3
1	A	220	GLU	2.3
1	C	249	VAL	2.3
1	F	237	TRP	2.3
1	F	78	ALA	2.3
1	G	201	ARG	2.3
1	H	197	ASN	2.3
1	B	96	VAL	2.3
1	D	108	ALA	2.3
1	G	78	ALA	2.3
1	G	247	ALA	2.3
1	A	266	LYS	2.3
1	F	126	PHE	2.3
1	G	115	PRO	2.3
1	H	158	ARG	2.3
1	H	107	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	70	ARG	2.2
1	G	225	LYS	2.2
1	H	265	VAL	2.2
1	H	240	LEU	2.2
1	E	246	TYR	2.2
1	E	227	ARG	2.2
1	A	263	ARG	2.2
1	C	39	HIS	2.2
1	G	244	ARG	2.2
1	D	256	LYS	2.2
1	H	176	PHE	2.2
1	D	226	ILE	2.2
1	D	5	ALA	2.2
1	E	126	PHE	2.2
1	C	260	VAL	2.2
1	H	86	SER	2.2
1	C	160	ASN	2.2
1	G	170	LEU	2.2
1	B	235	LYS	2.2
1	H	263	ARG	2.2
1	D	198	HIS	2.2
1	F	205	THR	2.2
1	B	101	VAL	2.2
1	E	167	ILE	2.2
1	H	105	TRP	2.2
1	F	195	ALA	2.2
1	A	8	LEU	2.2
1	G	264	LYS	2.2
1	B	138	TRP	2.1
1	F	117	ALA	2.1
1	G	79	VAL	2.1
1	C	88	ILE	2.1
1	D	140	ILE	2.1
1	D	105	TRP	2.1
1	A	55	LEU	2.1
1	A	226	ILE	2.1
1	B	191	LYS	2.1
1	F	2	LEU	2.1
1	H	260	VAL	2.1
1	H	152	GLY	2.1
1	F	30	ALA	2.1
1	D	146	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	241	VAL	2.1
1	A	199	PHE	2.1
1	G	120	THR	2.1
1	H	90	VAL	2.1
1	D	195	ALA	2.1
1	B	14	ILE	2.1
1	F	249	VAL	2.1
1	C	18	ALA	2.0
1	C	244	ARG	2.0
1	G	10	THR	2.0
1	B	176	PHE	2.0
1	D	265	VAL	2.0
1	B	258	ILE	2.0
1	E	106	ALA	2.0
1	H	201	ARG	2.0
1	A	147	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
6	ZN	B	301	1/1	0.81	0.24	0.66	201,201,201,201	0
6	ZN	A	301	1/1	0.96	0.30	0.49	160,160,160,160	0
6	ZN	H	301	1/1	0.97	0.29	-	178,178,178,178	0
7	W	B	319	1/1	0.89	0.53	-	274,274,274,274	1
7	W	B	310	1/1	0.99	0.62	-	185,185,185,185	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	W	B	307	1/1	0.98	0.56	-	139,139,139,139	1
7	W	F	306	1/1	0.99	0.56	-	176,176,176,176	0
7	W	F	304	1/1	0.99	0.59	-	164,164,164,164	1
7	W	A	304	1/1	0.92	0.38	-	241,241,241,241	1
7	W	F	309	1/1	0.98	0.54	-	179,179,179,179	1
7	W	A	303	1/1	0.74	0.44	-	240,240,240,240	1
6	ZN	C	301	1/1	0.84	0.19	-	237,237,237,237	0
6	ZN	E	301	1/1	0.80	0.32	-	164,164,164,164	0
7	W	B	305	1/1	0.97	0.55	-	239,239,239,239	0
7	W	F	302	1/1	0.99	0.54	-	178,178,178,178	1
6	ZN	D	301	1/1	0.81	0.10	-	220,220,220,220	0
7	W	A	305	1/1	-	-	-	265,265,265,265	1
6	ZN	F	301	1/1	0.93	0.11	-	236,236,236,236	0
7	W	B	321	1/1	0.91	0.23	-	228,228,228,228	1
7	W	F	310	1/1	0.99	0.59	-	178,178,178,178	1
7	W	B	302	1/1	0.99	0.58	-	146,146,146,146	1
7	W	B	309	1/1	1.00	0.53	-	159,159,159,159	1
7	W	B	304	1/1	0.99	0.52	-	185,185,185,185	1
7	W	B	312	1/1	0.98	0.54	-	148,148,148,148	1
7	W	F	312	1/1	0.99	0.59	-	166,166,166,166	1
7	W	F	307	1/1	0.99	0.53	-	155,155,155,155	1
7	W	B	306	1/1	0.97	0.55	-	210,210,210,210	0
7	W	B	308	1/1	0.99	0.55	-	181,181,181,181	1
7	W	B	303	1/1	1.00	0.55	-	159,159,159,159	1
7	W	F	308	1/1	1.00	0.57	-	236,236,236,236	0
7	W	B	314	1/1	0.89	0.29	-	227,227,227,227	1
6	ZN	G	302	1/1	0.60	0.19	-	277,277,277,277	0
7	W	F	305	1/1	0.99	0.56	-	173,173,173,173	1
7	W	B	316	1/1	0.95	0.41	-	235,235,235,235	1
7	W	B	318	1/1	0.93	0.35	-	224,224,224,224	1
7	W	B	315	1/1	0.76	0.41	-	249,249,249,249	1
7	W	G	301	1/1	0.99	0.56	-	185,185,185,185	0
7	W	F	311	1/1	0.99	0.63	-	237,237,237,237	0
7	W	F	303	1/1	0.99	0.54	-	179,179,179,179	1
7	W	B	311	1/1	0.97	0.58	-	167,167,167,167	1
7	W	A	302	1/1	0.95	0.48	-	307,307,307,307	1
7	W	B	313	1/1	0.98	0.55	-	184,184,184,184	1
7	W	B	317	1/1	0.92	0.27	-	224,224,224,224	1
7	W	B	320	1/1	0.97	0.49	-	302,302,302,302	1

6.5 Other polymers (i)

There are no such residues in this entry.