



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:24 AM UTC

PDB ID : 5C4X / pdb_00005c4x
Title : Crystal structure of a transcribing RNA Polymerase II complex reveals a complete transcription bubble
Authors : Barnes, C.O.; Calero, M.; Malik, I.; Spahr, H.; Zhang, Q.; Pullara, F.; Kaplan, C.D.; Calero, G.
Deposited on : 2015-06-18
Resolution : 4.00 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:

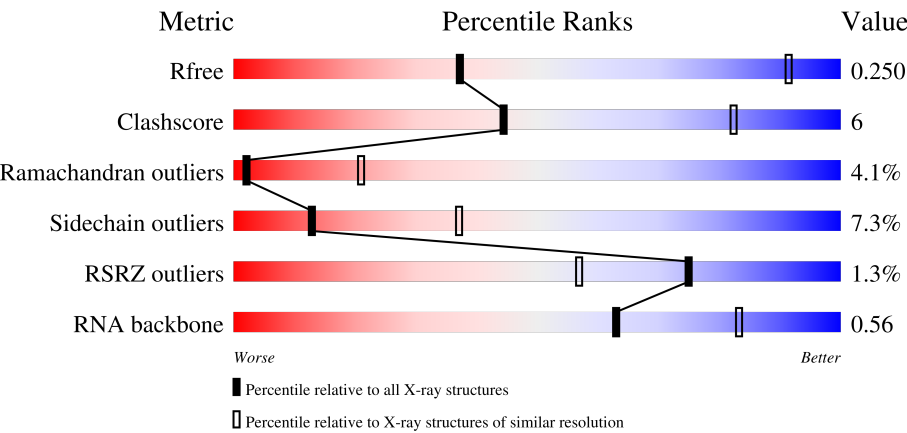
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 4.00 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.



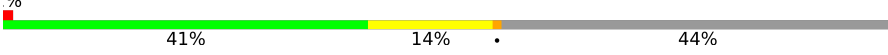
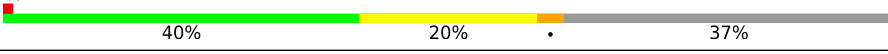
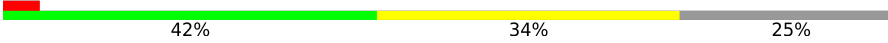
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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	1733	% 62% 18% • 17%
2	B	1224	2% 71% 22% • •
3	C	318	61% 19% • 17%
4	D	221	% 68% 12% • 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	179	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	9	
14	S	53	
15	U	53	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 33495 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1436	Total	C	N	O	S	0	0	0
			11280	7105	1972	2141	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1172	Total	C	N	O	S	0	0	0
			9293	5866	1630	1741	56			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2086	1312	347	414	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1417	875	254	286	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1339	861	222	248	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	LEU	-	expression tag	UNP P34087
G	173	GLU	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087
G	178	HIS	-	expression tag	UNP P34087
G	179	HIS	-	expression tag	UNP P34087

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	135	Total	C	N	O	S	0	0	0
			1080	679	182	214	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	114	Total	C	N	O	S	0	0	0
			921	568	165	178	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	66	Total	C	N	O	S	0	0	0
			540	345	94	95	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			

- Molecule 13 is a RNA chain called RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	9	Total	C	N	O	P	0	0	0
			197	88	40	60	9			

- Molecule 14 is a DNA chain called NON-TEMPLATE STRAND DNA (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	38	Total	C	N	O	P	0	0	0
			789	373	149	229	38			

- Molecule 15 is a DNA chain called TEMPLATE STRAND DNA (40-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	40	Total	C	N	O	P	0	0	0
			809	384	150	235	40			

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Zn	0	0
			2	2		
16	B	1	Total	Zn	0	0
			1	1		
16	C	2	Total	Zn	0	0
			2	2		
16	I	2	Total	Zn	0	0
			2	2		
16	J	1	Total	Zn	0	0
			1	1		
16	L	1	Total	Zn	0	0
			1	1		

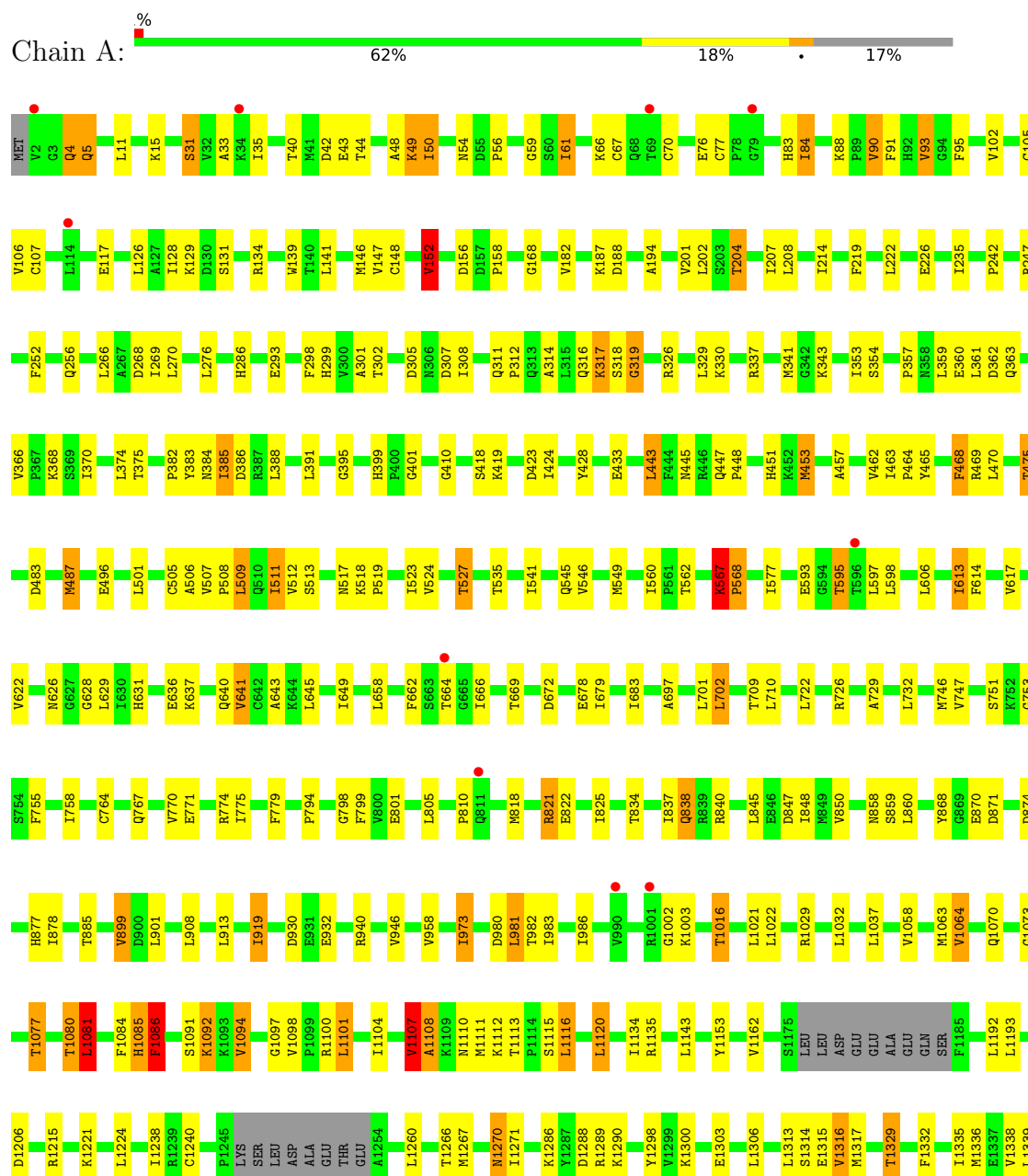
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

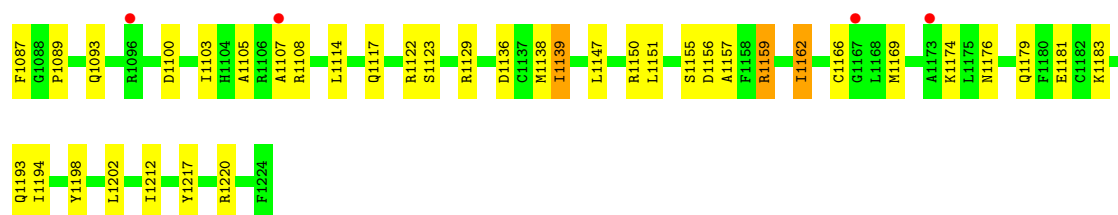
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Mg	0	0
			2	2		

3 Residue-property plots

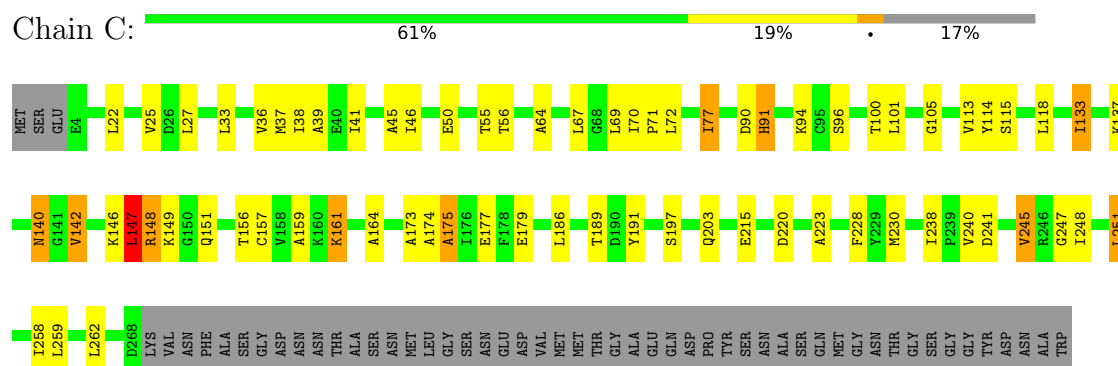
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

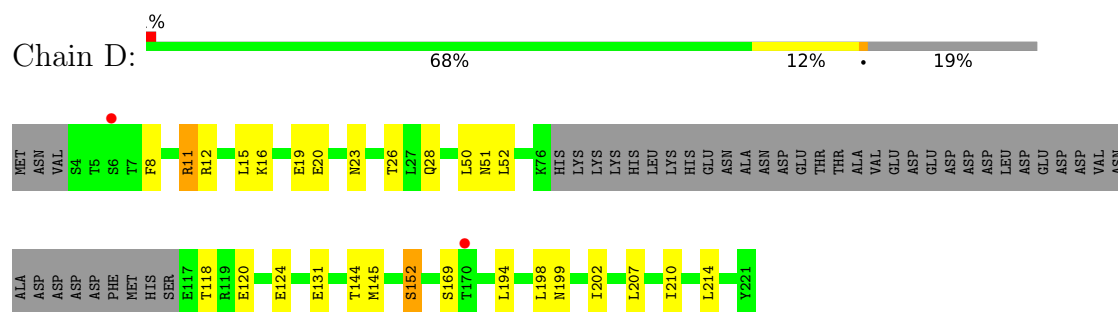




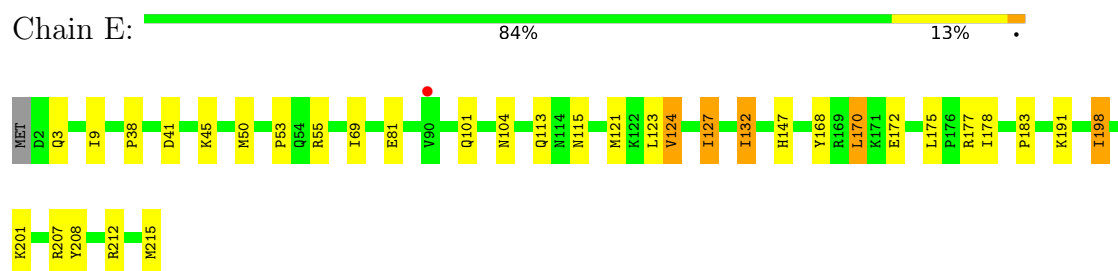
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



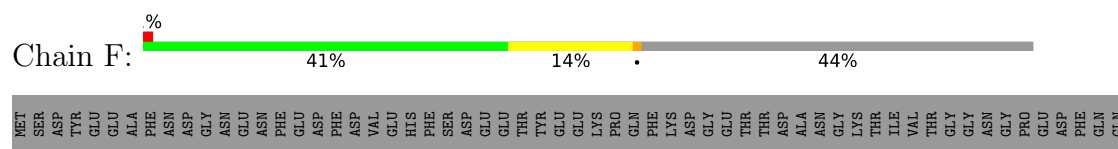
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

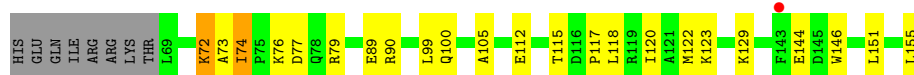


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

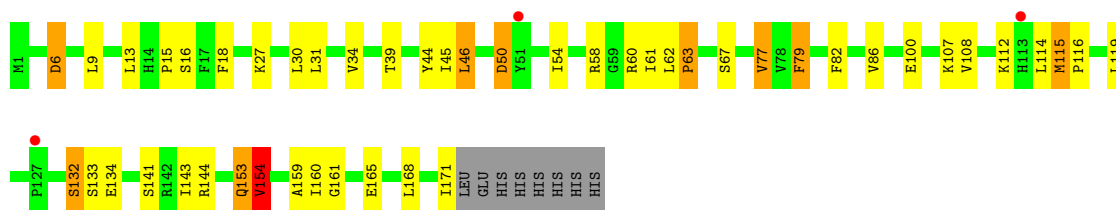


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

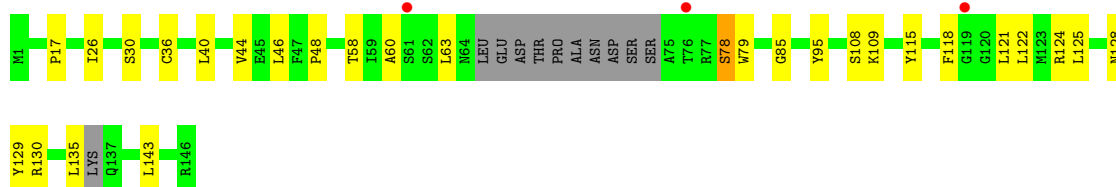
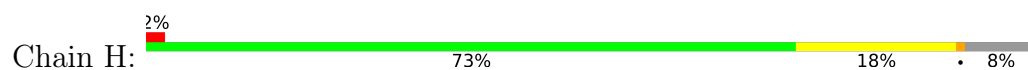




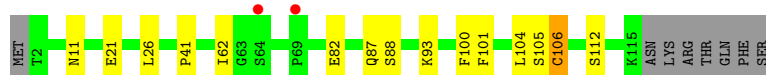
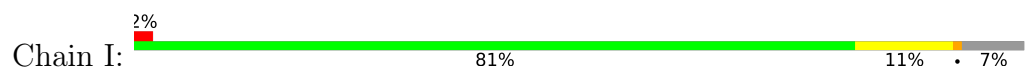
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



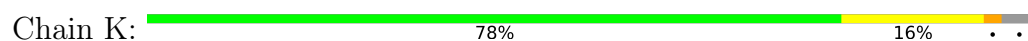
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4





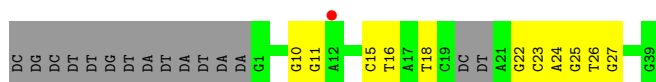
- Molecule 13: RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*A)-3')

Chain R: 89% 11%



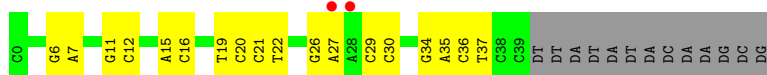
- Molecule 14: NON-TEMPLATE STRAND DNA (38-MER)

Chain S: 2% 51% 21% 28%



- Molecule 15: TEMPLATE STRAND DNA (40-MER)

Chain U: 4% 42% 34% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.79Å 393.36Å 281.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 40.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (40.00-4.00) 96.5 (40.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 4.00Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.210 , 0.227 0.232 , 0.250	Depositor DCC
R_{free} test set	2990 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	137.8	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 166.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.044 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	33495	wwPDB-VP
Average B, all atoms (Å ²)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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](#)

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

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	0.97	2/11485 (0.0%)	1.31	35/15536 (0.2%)
2	B	0.93	1/9470 (0.0%)	1.24	24/12770 (0.2%)
3	C	0.95	2/2124 (0.1%)	1.20	2/2879 (0.1%)
4	D	0.95	0/1427	1.23	2/1911 (0.1%)
5	E	0.94	1/1788 (0.1%)	1.19	4/2406 (0.2%)
6	F	0.89	0/717	1.18	0/967
7	G	0.92	0/1367	1.18	7/1844 (0.4%)
8	H	0.88	0/1097	1.09	0/1484
9	I	0.87	0/939	1.09	0/1266
10	J	0.93	0/549	1.21	1/738 (0.1%)
11	K	0.88	0/942	1.22	1/1272 (0.1%)
12	L	0.93	0/354	1.18	0/468
13	R	0.57	0/221	0.59	0/343
14	S	0.49	0/885	0.62	0/1364
15	U	0.50	0/906	0.87	6/1392 (0.4%)
All	All	0.92	6/34271 (0.0%)	1.22	82/46640 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	VAL	CA-C	6.61	1.59	1.52
2	B	923	GLU	CA-C	6.45	1.55	1.52
3	C	147	LEU	CA-C	6.28	1.60	1.52
1	A	50	ILE	CA-CB	5.96	1.60	1.54
5	E	124	VAL	CA-CB	5.11	1.57	1.54
3	C	148	ARG	N-CA	5.11	1.52	1.45

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1098	VAL	N-CA-CB	10.37	117.03	110.50
15	U	34	DG	O3'-P-O5'	9.98	118.97	104.00
15	U	34	DG	OP1-P-O3'	-9.44	79.69	108.00
15	U	34	DG	OP2-P-O3'	-9.11	80.66	108.00
15	U	35	DA	O5'-P-OP1	-9.03	81.92	109.00
15	U	35	DA	OP1-P-OP2	8.62	145.87	120.00
15	U	35	DA	O5'-P-OP2	-8.14	83.58	108.00
1	A	219	PHE	CA-CB-CG	7.71	121.51	113.80
1	A	1107	VAL	CA-C-N	7.56	135.31	121.70
1	A	1107	VAL	C-N-CA	7.56	135.31	121.70
2	B	332	ASP	CA-CB-CG	7.54	120.14	112.60
2	B	136	THR	CA-C-N	7.27	134.78	121.70
2	B	136	THR	C-N-CA	7.27	134.78	121.70
7	G	6	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	445	ASN	CA-CB-CG	7.12	119.72	112.60
2	B	930	ALA	CA-C-N	7.05	134.40	121.70
2	B	930	ALA	C-N-CA	7.05	134.40	121.70
1	A	1084	PHE	CA-CB-CG	6.99	120.79	113.80
2	B	79	THR	CA-C-N	6.88	134.09	121.70
2	B	79	THR	C-N-CA	6.88	134.09	121.70
2	B	221	ASN	CA-CB-CG	6.85	119.45	112.60
7	G	61	ILE	N-CA-CB	6.69	118.62	111.46
2	B	1139	ILE	N-CA-C	-6.61	104.21	110.42
2	B	436	VAL	N-CA-C	-6.58	106.31	112.83
1	A	252	PHE	CA-CB-CG	6.38	120.19	113.80
2	B	639	ILE	N-CA-CB	6.28	117.38	110.53
2	B	145	ARG	CA-C-N	6.24	132.93	121.70
2	B	145	ARG	C-N-CA	6.24	132.93	121.70
1	A	463	ILE	N-CA-C	6.19	114.71	107.84
1	A	641	VAL	N-CA-C	-6.16	104.50	110.72
1	A	1086	PHE	CA-C-N	6.12	132.71	121.70
1	A	1086	PHE	C-N-CA	6.12	132.71	121.70
4	D	28	GLN	N-CA-C	-6.10	101.11	109.71
7	G	45	ILE	N-CA-CB	5.88	117.70	111.00
10	J	3	VAL	N-CA-CB	5.88	119.44	111.21
1	A	798	GLY	N-CA-C	5.86	123.99	115.32
2	B	344	LYS	CA-C-N	5.86	132.72	121.54
2	B	344	LYS	C-N-CA	5.86	132.72	121.54
1	A	307	ASP	CA-C-N	5.84	132.22	121.70
1	A	307	ASP	C-N-CA	5.84	132.22	121.70
2	B	557	PHE	CA-CB-CG	5.82	119.62	113.80
5	E	123	LEU	CA-C-N	5.78	124.95	120.33
5	E	123	LEU	C-N-CA	5.78	124.95	120.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	507	VAL	N-CA-CB	5.73	114.36	110.52
4	D	26	THR	N-CA-C	-5.63	105.72	112.59
3	C	147	LEU	N-CA-C	5.63	118.25	109.52
1	A	317	LYS	CA-C-N	5.54	131.68	121.70
1	A	317	LYS	C-N-CA	5.54	131.68	121.70
2	B	694	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	930	ASP	N-CA-C	-5.52	104.66	111.40
1	A	871	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	48	ALA	CA-C-N	5.48	132.00	121.54
1	A	48	ALA	C-N-CA	5.48	132.00	121.54
7	G	18	PHE	CA-CB-CG	5.39	119.19	113.80
5	E	147	HIS	CA-C-N	5.33	127.37	120.44
5	E	147	HIS	C-N-CA	5.33	127.37	120.44
11	K	63	VAL	N-CA-CB	5.25	117.35	111.89
1	A	1329	THR	N-CA-CB	5.23	117.96	110.06
2	B	1013	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	1097	GLY	CA-C-N	5.22	123.53	120.24
1	A	1097	GLY	C-N-CA	5.22	123.53	120.24
3	C	140	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	319	GLY	N-CA-C	5.21	125.52	113.18
1	A	1063	MET	CA-C-N	5.19	131.32	121.97
1	A	1063	MET	C-N-CA	5.19	131.32	121.97
7	G	77	VAL	N-CA-CB	5.18	117.71	110.56
2	B	150	GLU	CA-C-N	5.17	131.00	121.70
2	B	150	GLU	C-N-CA	5.17	131.00	121.70
1	A	475	THR	CA-C-N	5.14	126.16	119.78
1	A	475	THR	C-N-CA	5.14	126.16	119.78
1	A	1002	GLY	N-CA-C	5.14	119.59	110.80
2	B	1041	GLU	CA-C-N	5.12	124.96	120.10
2	B	1041	GLU	C-N-CA	5.12	124.96	120.10
1	A	973	ILE	N-CA-CB	5.11	116.10	110.53
1	A	613	ILE	N-CA-C	-5.10	106.82	111.67
7	G	50	ASP	CA-CB-CG	5.09	117.69	112.60
2	B	1006	ILE	N-CA-CB	5.08	116.06	110.53
2	B	97	VAL	N-CA-CB	5.05	116.76	111.00
1	A	31	SER	N-CA-C	5.03	116.78	110.24
7	G	79	PHE	CA-CB-CG	5.01	118.81	113.80
1	A	517	ASN	CA-CB-CG	5.00	117.60	112.60

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	11280	0	11325	165	0
2	B	9293	0	9282	134	0
3	C	2086	0	2045	43	0
4	D	1417	0	1428	6	0
5	E	1752	0	1776	14	0
6	F	705	0	731	12	0
7	G	1339	0	1357	21	0
8	H	1080	0	1049	12	0
9	I	921	0	870	7	0
10	J	540	0	554	9	0
11	K	924	0	934	9	0
12	L	352	0	378	4	0
13	R	197	0	97	1	0
14	S	789	0	429	8	0
15	U	809	0	447	11	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	2	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	2	0	0	0	0
All	All	33495	0	32702	395	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 6.

All (395) 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:697:ALA:HA	1:A:702:LEU:HD11	1.42	1.01
14:S:25:DG:H4'	14:S:26:DT:H5'	1.43	1.00
3:C:148:ARG:NH2	10:J:65:PRO:HD3	1.76	0.99
3:C:146:LYS:C	3:C:147:LEU:HD12	1.92	0.95
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.48	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:MET:HE1	2:B:1015:HIS:HA	1.47	0.93
2:B:145:ARG:HA	2:B:146:GLU:HB2	1.58	0.85
15:U:29:DC:H1'	15:U:30:DC:H5	1.42	0.84
2:B:100:PRO:HG3	2:B:172:ILE:HG21	1.63	0.80
2:B:919:SER:HB2	2:B:920:PRO:HA	1.65	0.79
3:C:77:ILE:HD13	3:C:161:LYS:HE3	1.66	0.78
1:A:105:CYS:SG	1:A:139:TRP:HA	2.24	0.76
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.49	0.75
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.67	0.75
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.70	0.73
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.69	0.73
2:B:145:ARG:HA	2:B:146:GLU:CB	2.18	0.73
2:B:867:GLY:HA3	2:B:868:MET:HB3	1.70	0.73
1:A:746:MET:CE	2:B:1015:HIS:HA	2.17	0.72
1:A:913:LEU:HD11	1:A:982:THR:HA	1.72	0.72
2:B:994:TYR:HB2	2:B:999:MET:HE3	1.71	0.71
2:B:79:THR:HA	2:B:81:SER:N	2.06	0.71
14:S:25:DG:C4'	14:S:26:DT:H5'	2.19	0.70
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.27	0.69
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.75	0.68
1:A:311:GLN:HG2	1:A:312:PRO:HD3	1.76	0.68
15:U:15:DA:H2''	15:U:16:DC:O5'	1.94	0.67
14:S:15:DC:H2''	14:S:16:DT:H5''	1.76	0.67
11:K:42:LEU:HD23	11:K:46:ILE:HD11	1.76	0.67
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.77	0.67
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.77	0.66
1:A:512:VAL:HA	1:A:519:PRO:HA	1.78	0.66
5:E:124:VAL:HG13	5:E:132:ILE:HG23	1.77	0.66
3:C:147:LEU:HD12	3:C:147:LEU:N	2.10	0.65
3:C:113:VAL:HG23	3:C:147:LEU:HD13	1.78	0.65
2:B:84:ILE:HG22	2:B:140:ILE:HG12	1.79	0.64
1:A:1107:VAL:HG11	1:A:1381:LEU:HD23	1.80	0.64
6:F:117:PRO:HA	6:F:120:ILE:HD12	1.80	0.63
14:S:22:DG:H4'	14:S:24:DA:H2''	1.79	0.63
1:A:567:LYS:HG2	1:A:568:PRO:HD3	1.81	0.63
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.80	0.63
3:C:148:ARG:O	3:C:149:LYS:C	2.41	0.62
2:B:867:GLY:CA	2:B:868:MET:HB3	2.29	0.62
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.82	0.62
1:A:370:ILE:HD12	2:B:1105:ALA:HB2	1.80	0.62
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:HG3	1:A:1381:LEU:HD13	1.82	0.61
15:U:29:DC:H1'	15:U:30:DC:C5	2.32	0.61
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.82	0.61
1:A:549:MET:HG2	1:A:577:ILE:HD12	1.83	0.61
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.30	0.61
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.82	0.61
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.40	0.60
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.82	0.60
15:U:11:DG:H2''	15:U:12:DC:O5'	2.02	0.60
1:A:1081:LEU:HD11	1:A:1085:HIS:HB2	1.83	0.60
1:A:88:LYS:HD3	1:A:293:GLU:HG3	1.83	0.59
1:A:1107:VAL:HA	1:A:1108:ALA:HB3	1.84	0.59
1:A:448:PRO:HB3	15:U:19:DT:H1'	1.84	0.59
3:C:148:ARG:NH2	10:J:65:PRO:CD	2.60	0.59
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.35	0.59
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.38	0.59
2:B:1082:MET:HA	3:C:189:THR:HA	1.84	0.59
1:A:40:THR:O	1:A:49:LYS:HG2	2.03	0.59
1:A:341:MET:HE1	1:A:1425:SER:HA	1.84	0.59
1:A:1080:THR:O	1:A:1081:LEU:HB3	2.02	0.59
7:G:9:LEU:HD23	7:G:30:LEU:HD12	1.83	0.59
1:A:31:SER:HB2	1:A:83:HIS:HB3	1.85	0.58
2:B:1008:PRO:HB3	2:B:1087:PHE:HE2	1.68	0.58
3:C:113:VAL:CG2	3:C:147:LEU:HD13	2.34	0.58
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.84	0.57
3:C:258:ILE:HG13	11:K:19:LEU:HD11	1.85	0.57
1:A:1313:LEU:HD23	1:A:1338:VAL:HG11	1.86	0.57
1:A:519:PRO:HD3	1:A:631:HIS:HD2	1.69	0.57
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.87	0.57
1:A:354:SER:HB2	1:A:469:ARG:HG2	1.87	0.57
1:A:1336:MET:HE2	1:A:1381:LEU:HB2	1.86	0.56
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.87	0.56
4:D:23:ASN:HB3	7:G:82:PHE:HD1	1.70	0.56
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.88	0.56
2:B:1129:ARG:HG2	15:U:20:DC:H5''	1.86	0.56
1:A:1444:MET:HB3	7:G:58:ARG:HB3	1.88	0.56
2:B:245:GLU:N	2:B:246:LYS:HA	2.20	0.55
1:A:317:LYS:HA	1:A:318:SER:C	2.31	0.55
3:C:46:ILE:HA	3:C:159:ALA:HA	1.87	0.55
5:E:124:VAL:HG22	5:E:132:ILE:HD13	1.89	0.55
5:E:38:PRO:HD2	5:E:41:ASP:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:CYS:HA	2:B:67:SER:HB2	1.89	0.55
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.88	0.55
3:C:71:PRO:HB2	3:C:133:ILE:HB	1.88	0.55
1:A:382:PRO:HD3	1:A:428:TYR:HE2	1.71	0.55
2:B:251:ILE:HB	14:S:18:DT:H5'	1.87	0.55
6:F:146:TRP:HB3	6:F:151:LEU:HD11	1.89	0.55
2:B:129:PHE:HB3	2:B:164:LYS:HB3	1.89	0.55
2:B:161:GLU:HG2	2:B:162:SER:H	1.71	0.55
2:B:477:ALA:HB3	13:R:6:G:H5'	1.89	0.54
1:A:679:ILE:HG13	1:A:732:LEU:HD23	1.89	0.54
1:A:266:LEU:HA	1:A:269:ILE:HD12	1.88	0.54
7:G:119:LEU:HD12	7:G:132:SER:HB2	1.89	0.54
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.73	0.54
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.72	0.54
2:B:640:VAL:HA	2:B:651:LEU:HA	1.89	0.54
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.89	0.54
1:A:464:PRO:HB2	11:K:4:PRO:HD3	1.90	0.54
1:A:506:ALA:HB3	1:A:509:LEU:HB2	1.90	0.54
1:A:810:PRO:HB3	2:B:745:PRO:HB3	1.90	0.54
2:B:655:LYS:O	2:B:658:ILE:HG22	2.07	0.54
2:B:1122:ARG:HD3	15:U:22:DT:H5''	1.89	0.54
1:A:669:THR:HG23	1:A:805:LEU:HD13	1.90	0.54
1:A:709:THR:HG21	9:I:93:LYS:O	2.07	0.54
3:C:148:ARG:CZ	10:J:65:PRO:HD3	2.37	0.54
1:A:946:VAL:HG22	5:E:201:LYS:HB3	1.89	0.53
14:S:23:DC:H2''	14:S:24:DA:OP2	2.09	0.53
15:U:36:DC:H2''	15:U:37:DT:C6	2.43	0.53
1:A:874:ASP:HB3	1:A:877:HIS:CD2	2.42	0.53
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.90	0.53
2:B:860:MET:HB3	2:B:965:LYS:HE3	1.90	0.53
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.89	0.53
1:A:4:GLN:O	1:A:5:GLN:HB2	2.08	0.53
1:A:508:PRO:HA	1:A:511:ILE:HG12	1.90	0.53
1:A:1224:LEU:HD21	1:A:1240:CYS:HB3	1.91	0.53
1:A:908:LEU:HD21	1:A:1029:ARG:HG2	1.89	0.53
1:A:567:LYS:HG3	8:H:95:TYR:HA	1.91	0.52
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.91	0.52
3:C:147:LEU:N	3:C:147:LEU:CD1	2.73	0.52
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.40	0.52
1:A:1091:SER:O	1:A:1092:LYS:HB2	2.09	0.52
1:A:981:LEU:HD13	1:A:986:ILE:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:GLY:HA2	2:B:146:GLU:HB2	1.91	0.52
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.90	0.52
2:B:806:THR:HG23	2:B:1045:SER:HA	1.91	0.52
3:C:33:LEU:HG	3:C:37:MET:HE2	1.91	0.52
1:A:821:ARG:HD3	2:B:527:THR:HG21	1.92	0.51
1:A:360:GLU:HB3	1:A:363:GLN:HB2	1.93	0.51
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.92	0.51
2:B:134:LYS:HD3	2:B:159:ASP:HB3	1.93	0.51
1:A:451:HIS:HA	1:A:1070:GLN:HB3	1.93	0.51
1:A:560:ILE:HD12	8:H:78:SER:HB2	1.93	0.51
2:B:387:LEU:HD23	2:B:393:LYS:HB2	1.91	0.51
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.10	0.51
1:A:316:GLN:O	1:A:318:SER:O	2.27	0.51
2:B:711:GLU:HB3	2:B:712:PRO:HD3	1.93	0.51
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.92	0.51
1:A:1420:ASP:HB2	1:A:1422:ARG:HG2	1.93	0.51
3:C:70:ILE:HD12	3:C:142:VAL:HG11	1.93	0.51
2:B:1138:MET:HB2	2:B:1147:LEU:HD12	1.93	0.51
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.93	0.51
2:B:824:ILE:HA	2:B:1089:PRO:HA	1.93	0.51
2:B:867:GLY:HA3	2:B:868:MET:CB	2.38	0.51
1:A:770:VAL:HG23	1:A:822:GLU:HG3	1.93	0.51
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.93	0.51
3:C:113:VAL:CG2	3:C:147:LEU:CD1	2.89	0.51
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.41	0.50
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.92	0.50
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.93	0.50
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.46	0.50
1:A:353:ILE:CG2	1:A:487:MET:HB2	2.42	0.50
3:C:113:VAL:HG23	3:C:147:LEU:CD1	2.41	0.50
1:A:208:LEU:HD13	1:A:235:ILE:HB	1.93	0.50
2:B:1162:ILE:HG22	2:B:1169:MET:HG3	1.94	0.50
3:C:105:GLY:O	3:C:149:LYS:HA	2.12	0.50
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.94	0.50
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.93	0.50
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.47	0.49
1:A:702:LEU:HB2	1:A:710:LEU:HD11	1.93	0.49
1:A:834:THR:HG21	1:A:1077:THR:HA	1.95	0.49
2:B:100:PRO:HG3	2:B:172:ILE:CG2	2.39	0.49
3:C:77:ILE:HD11	3:C:161:LYS:HG3	1.94	0.49
8:H:58:THR:HB	8:H:143:LEU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.94	0.49
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.94	0.49
3:C:36:VAL:HG11	3:C:251:LEU:HD12	1.95	0.49
2:B:125:SER:HA	2:B:171:PRO:HA	1.94	0.49
2:B:161:GLU:HG3	2:B:165:VAL:CG1	2.42	0.49
2:B:888:GLY:O	2:B:909:ASP:HA	2.12	0.49
5:E:178:ILE:HB	5:E:212:ARG:HD3	1.95	0.49
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.95	0.49
6:F:74:ILE:HB	6:F:144:GLU:HG2	1.93	0.49
7:G:44:TYR:HB2	7:G:79:PHE:HB3	1.95	0.49
11:K:12:LEU:HA	11:K:37:LYS:HD2	1.94	0.49
1:A:658:LEU:HD13	2:B:831:SER:HB3	1.94	0.48
1:A:755:PHE:HA	1:A:758:ILE:HD12	1.95	0.48
6:F:118:LEU:HG	6:F:122:MET:HE2	1.95	0.48
2:B:745:PRO:HB2	2:B:1047:PHE:CD2	2.49	0.48
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.78	0.48
1:A:598:LEU:HD11	8:H:124:ARG:HB2	1.95	0.48
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.94	0.48
2:B:930:ALA:HA	2:B:931:TYR:C	2.39	0.48
3:C:259:LEU:HA	3:C:262:LEU:HD12	1.96	0.48
1:A:443:LEU:HD23	1:A:501:LEU:HD21	1.96	0.48
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	1.95	0.48
2:B:559:SER:HA	2:B:563:MET:HB2	1.96	0.48
6:F:105:ALA:HA	7:G:16:SER:HA	1.96	0.48
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.96	0.48
1:A:383:TYR:HB3	6:F:115:THR:HA	1.96	0.48
1:A:523:ILE:HD13	1:A:622:VAL:HG22	1.96	0.48
2:B:526:GLU:HG3	2:B:771:SER:HB2	1.95	0.48
2:B:848:ARG:HA	3:C:69:LEU:HD21	1.95	0.48
6:F:76:LYS:HA	6:F:79:ARG:CZ	2.44	0.48
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.95	0.47
1:A:1116:LEU:HB2	1:A:1329:THR:HA	1.95	0.47
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.97	0.47
2:B:855:PHE:HB3	2:B:970:THR:HB	1.95	0.47
2:B:693:ILE:HG23	2:B:697:GLU:HB3	1.96	0.47
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.96	0.47
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.50	0.47
1:A:1266:THR:O	1:A:1270:ASN:HB3	2.14	0.47
2:B:367:LEU:HB2	2:B:370:PHE:HE2	1.80	0.47
2:B:619:ILE:HD13	9:I:62:ILE:HA	1.97	0.47
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:90:ARG:HD2	6:F:155:LEU:HD22	1.97	0.47
1:A:106:VAL:HG11	1:A:214:ILE:HG12	1.96	0.47
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.96	0.47
1:A:1332:PHE:HA	1:A:1335:ILE:HD12	1.97	0.47
2:B:101:MET:HG2	2:B:111:ALA:HA	1.96	0.47
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.96	0.47
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.95	0.47
1:A:95:PHE:HZ	2:B:1212:ILE:HD11	1.80	0.46
1:A:496:GLU:HB2	6:F:99:LEU:HD12	1.96	0.46
1:A:15:LYS:O	1:A:1421:CYS:HB2	2.15	0.46
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.97	0.46
2:B:63:ILE:HG23	2:B:92:PHE:HB2	1.97	0.46
2:B:95:ILE:HA	2:B:129:PHE:O	2.15	0.46
2:B:705:MET:HE3	2:B:742:GLU:HG2	1.96	0.46
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.97	0.46
5:E:177:ARG:HG2	5:E:215:MET:HE3	1.97	0.46
8:H:125:LEU:HG	8:H:130:ARG:HH21	1.79	0.46
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.97	0.46
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.97	0.46
1:A:359:LEU:HD22	1:A:363:GLN:HB3	1.97	0.46
2:B:1002:THR:HG23	2:B:1072:MET:HE3	1.97	0.46
1:A:70:CYS:HB2	2:B:1174:LYS:HG2	1.98	0.46
2:B:703:ILE:HA	2:B:740:HIS:O	2.16	0.46
10:J:14:VAL:HA	10:J:17:LYS:HD3	1.97	0.46
4:D:52:LEU:HD13	4:D:152:SER:HA	1.97	0.46
7:G:100:GLU:HB3	7:G:107:LYS:HG2	1.97	0.46
2:B:130:VAL:O	2:B:165:VAL:HG22	2.16	0.46
2:B:283:VAL:HG23	2:B:297:ILE:HG21	1.98	0.46
14:S:26:DT:H5''	14:S:27:DG:H5'	1.97	0.46
1:A:102:VAL:HG22	1:A:222:LEU:HD23	1.98	0.46
1:A:678:GLU:HB3	1:A:732:LEU:HD21	1.96	0.46
11:K:77:THR:HB	11:K:81:TYR:HD2	1.81	0.46
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.98	0.45
1:A:1317:MET:HE1	1:A:1339:LEU:HD21	1.98	0.45
2:B:856:PHE:HB3	2:B:967:ARG:HD2	1.98	0.45
15:U:6:DG:C2'	15:U:7:DA:O5'	2.64	0.45
1:A:451:HIS:CD2	1:A:453:MET:HE3	2.51	0.45
12:L:31:CYS:HA	12:L:56:LEU:HA	1.97	0.45
1:A:859:SER:O	1:A:1422:ARG:HD3	2.16	0.45
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.98	0.45
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:THR:HA	2:B:137:TYR:CB	2.47	0.45
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.98	0.45
2:B:298:LEU:HD12	2:B:311:LEU:HD23	1.98	0.45
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.97	0.45
2:B:212:LEU:HD23	2:B:479:VAL:HG12	1.98	0.45
5:E:168:TYR:HB3	5:E:170:LEU:HD12	1.97	0.45
1:A:847:ASP:HB2	1:A:858:ASN:HB2	1.99	0.45
1:A:1101:LEU:HA	1:A:1104:ILE:HD12	1.99	0.45
1:A:546:VAL:HG23	1:A:577:ILE:HG21	1.99	0.45
1:A:821:ARG:NH1	2:B:534:GLY:HA2	2.32	0.45
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.99	0.45
2:B:79:THR:HA	2:B:80:GLU:C	2.42	0.45
3:C:91:HIS:HB2	3:C:96:SER:OG	2.16	0.45
8:H:125:LEU:HG	8:H:130:ARG:NH2	2.32	0.45
1:A:242:PRO:HD2	1:A:266:LEU:HD11	1.99	0.45
1:A:606:LEU:HB3	1:A:613:ILE:HB	1.99	0.45
2:B:338:GLY:HA2	2:B:339:THR:HA	1.64	0.45
2:B:798:TYR:HB3	10:J:4:PRO:HG3	1.99	0.45
7:G:46:LEU:HB2	7:G:77:VAL:HG23	1.99	0.45
2:B:301:ILE:HD13	2:B:379:GLY:HA2	1.99	0.44
2:B:205:ILE:HG21	2:B:462:ALA:HB2	1.98	0.44
1:A:598:LEU:HD21	8:H:115:TYR:HD1	1.82	0.44
5:E:178:ILE:HB	5:E:212:ARG:HB3	2.00	0.44
1:A:326:ARG:NH2	1:A:330:LYS:HE2	2.33	0.44
2:B:424:LEU:HD12	2:B:449:ASN:HB3	1.99	0.44
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	2.00	0.44
4:D:11:ARG:HA	4:D:12:ARG:HA	1.79	0.44
5:E:101:GLN:HB2	5:E:127:ILE:HD13	1.99	0.44
9:I:88:SER:HA	9:I:100:PHE:HE2	1.81	0.44
1:A:818:MET:HG3	2:B:514:LEU:HD23	2.00	0.44
1:A:1290:LYS:HG2	1:A:1298:TYR:HB3	1.99	0.44
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.99	0.44
2:B:878:GLN:HB2	2:B:881:ASN:HB2	2.00	0.44
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.99	0.44
1:A:374:LEU:HA	2:B:1107:ALA:HB2	2.00	0.44
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.53	0.44
1:A:1288:ASP:HB3	1:A:1300:LYS:HG2	1.99	0.44
2:B:246:LYS:HE3	2:B:249:ARG:HA	1.99	0.44
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.83	0.44
7:G:62:LEU:HD12	7:G:67:SER:HB2	1.99	0.44
8:H:30:SER:HB3	8:H:36:CYS:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:HB3	2:B:261:ARG:HG2	2.00	0.43
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.00	0.43
3:C:115:SER:O	3:C:118:LEU:HG	2.18	0.43
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.99	0.43
1:A:722:LEU:HD21	1:A:794:PRO:HB3	2.00	0.43
3:C:114:TYR:CG	3:C:140:ASN:HB2	2.53	0.43
3:C:259:LEU:HD12	11:K:91:CYS:HB3	2.00	0.43
5:E:55:ARG:NH1	5:E:113:GLN:HG3	2.33	0.43
1:A:90:VAL:HA	1:A:204:THR:HG21	1.99	0.43
9:I:105:SER:O	9:I:106:CYS:HB3	2.19	0.43
1:A:562:THR:HG22	8:H:79:TRP:HD1	1.82	0.43
1:A:874:ASP:HB3	1:A:877:HIS:HD2	1.82	0.43
2:B:130:VAL:HG13	2:B:132:VAL:HG23	2.01	0.43
2:B:319:GLU:HA	2:B:322:PHE:HB2	2.00	0.43
10:J:44:TYR:HA	10:J:47:ARG:HB2	2.01	0.43
2:B:863:GLU:HB3	2:B:961:LEU:HD22	2.00	0.43
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.99	0.43
2:B:118:ARG:HG3	2:B:204:ILE:HD13	2.01	0.43
3:C:64:ALA:HA	3:C:67:LEU:HD12	2.00	0.43
12:L:30:ILE:HG13	12:L:57:LEU:HB2	2.00	0.43
1:A:84:ILE:HD13	1:A:84:ILE:HA	1.85	0.43
1:A:361:LEU:HD21	1:A:511:ILE:HD11	1.99	0.43
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.00	0.43
3:C:41:ILE:HD11	3:C:247:GLY:HA2	2.01	0.43
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.01	0.43
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.01	0.43
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.00	0.43
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.01	0.43
1:A:126:LEU:HD23	1:A:134:ARG:HD2	2.01	0.43
4:D:202:ILE:HG21	4:D:207:LEU:HD13	2.00	0.43
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.59	0.42
1:A:1193:LEU:HD12	1:A:1260:LEU:HG	2.00	0.42
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.01	0.42
2:B:211:VAL:HG21	2:B:483:LEU:HD13	2.01	0.42
7:G:108:VAL:HG22	7:G:159:ALA:HB3	2.01	0.42
9:I:82:GLU:HG2	9:I:104:LEU:HD23	2.02	0.42
2:B:218:SER:HA	2:B:404:LYS:HG2	2.01	0.42
2:B:1100:ASP:HA	2:B:1103:ILE:HG22	2.01	0.42
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.00	0.42
3:C:25:VAL:HB	3:C:228:PHE:HE2	1.85	0.42
3:C:148:ARG:HB3	3:C:151:GLN:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.54	0.42
1:A:302:THR:HA	1:A:305:ASP:O	2.20	0.42
1:A:523:ILE:HG23	1:A:527:THR:HB	2.01	0.42
1:A:834:THR:HG21	1:A:1077:THR:CA	2.49	0.42
2:B:780:VAL:HG12	2:B:795:ILE:HG13	2.02	0.42
15:U:26:DG:H4'	15:U:27:DA:OP1	2.20	0.42
1:A:541:ILE:HG23	1:A:545:GLN:HB3	2.02	0.42
1:A:885:THR:HG22	1:A:940:ARG:HB2	2.02	0.42
2:B:363:HIS:HD2	2:B:364:ILE:HG13	1.84	0.42
7:G:153:GLN:HG2	7:G:154:VAL:HG23	2.02	0.42
10:J:57:ILE:HG13	10:J:61:LEU:HD23	2.02	0.42
14:S:10:DG:H2''	14:S:11:DG:O5'	2.19	0.42
2:B:878:GLN:HB2	2:B:881:ASN:CB	2.49	0.42
2:B:950:ASP:O	2:B:967:ARG:HB3	2.20	0.42
1:A:747:VAL:HG22	1:A:753:GLY:HA3	2.01	0.42
2:B:842:ASN:O	2:B:846:ILE:HG12	2.20	0.42
2:B:1114:LEU:O	2:B:1198:TYR:HE2	2.03	0.42
1:A:451:HIS:CD2	1:A:453:MET:HB2	2.55	0.42
1:A:1100:ARG:HG3	1:A:1104:ILE:HD11	2.01	0.42
1:A:1345:ARG:HB3	1:A:1376:THR:HG21	2.01	0.41
2:B:901:PRO:HD3	12:L:58:LYS:HB3	2.02	0.41
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.02	0.41
1:A:726:ARG:HG2	1:A:764:CYS:HB3	2.01	0.41
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	2.00	0.41
1:A:395:GLY:O	1:A:401:GLY:HA3	2.20	0.41
2:B:87:LYS:HB2	2:B:137:TYR:HD2	1.85	0.41
1:A:33:ALA:HB1	1:A:56:PRO:HG2	2.03	0.41
1:A:182:VAL:HG12	1:A:201:VAL:HA	2.02	0.41
1:A:567:LYS:CB	1:A:568:PRO:CD	2.95	0.41
1:A:343:LYS:HD2	2:B:1155:SER:OG	2.20	0.41
1:A:384:ASN:O	1:A:386:ASP:N	2.54	0.41
1:A:1368:MET:HE3	1:A:1368:MET:HB2	1.98	0.41
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.02	0.41
3:C:50:GLU:HB2	3:C:156:THR:HB	2.02	0.41
1:A:818:MET:HA	2:B:514:LEU:HB3	2.01	0.41
2:B:868:MET:HG3	2:B:869:SER:N	2.35	0.41
2:B:778:MET:SD	2:B:794:ASN:HB3	2.61	0.41
7:G:144:ARG:HG2	7:G:168:LEU:HD23	2.02	0.41
15:U:20:DC:H2'	15:U:21:DC:O4'	2.20	0.41
1:A:366:VAL:HG22	1:A:468:PHE:HE1	1.86	0.41
1:A:368:LYS:HA	1:A:462:VAL:CG1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:GLN:HA	1:A:799:PHE:HA	2.03	0.41
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.50	0.41
2:B:825:VAL:HG23	2:B:1010:LEU:HG	2.03	0.41
2:B:961:LEU:HB3	2:B:962:LYS:H	1.73	0.41
3:C:46:ILE:HG12	3:C:157:CYS:HB3	2.02	0.41
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.02	0.41
5:E:9:ILE:HG12	5:E:53:PRO:HG3	2.03	0.41
7:G:114:LEU:HD23	7:G:161:GLY:O	2.21	0.41
11:K:58:PHE:HE1	11:K:74:ARG:HB3	1.85	0.41
1:A:1453:TYR:HB3	6:F:129:LYS:HE2	2.03	0.41
1:A:845:LEU:HA	1:A:848:ILE:HD12	2.03	0.40
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.51	0.40
3:C:220:ASP:HB3	3:C:223:ALA:HB2	2.04	0.40
11:K:20:LYS:HB2	11:K:34:THR:HB	2.04	0.40
2:B:420:LEU:HD21	2:B:456:GLY:HA3	2.03	0.40
3:C:177:GLU:O	3:C:230:MET:HB2	2.22	0.40
1:A:722:LEU:HD23	1:A:767:GLN:HB2	2.04	0.40
6:F:100:GLN:HG2	7:G:15:PRO:HB3	2.03	0.40
1:A:645:LEU:O	1:A:649:ILE:HG12	2.22	0.40
1:A:1313:LEU:HA	1:A:1316:VAL:HG12	2.03	0.40
2:B:754:SER:HB2	2:B:812:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1430/1733 (82%)	1225 (86%)	144 (10%)	61 (4%)	2	20
2	B	1158/1224 (95%)	963 (83%)	142 (12%)	53 (5%)	2	20
3	C	263/318 (83%)	231 (88%)	25 (10%)	7 (3%)	4	28
4	D	174/221 (79%)	149 (86%)	15 (9%)	10 (6%)	1	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	212/215 (99%)	196 (92%)	9 (4%)	7 (3%)	3	24
6	F	85/155 (55%)	75 (88%)	8 (9%)	2 (2%)	4	30
7	G	169/179 (94%)	142 (84%)	21 (12%)	6 (4%)	2	23
8	H	129/146 (88%)	108 (84%)	13 (10%)	8 (6%)	1	15
9	I	112/122 (92%)	100 (89%)	9 (8%)	3 (3%)	4	28
10	J	64/70 (91%)	54 (84%)	9 (14%)	1 (2%)	7	37
11	K	113/120 (94%)	106 (94%)	6 (5%)	1 (1%)	14	48
12	L	42/70 (60%)	30 (71%)	9 (21%)	3 (7%)	1	14
All	All	3951/4573 (86%)	3379 (86%)	410 (10%)	162 (4%)	2	21

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	66	LYS
1	A	76	GLU
1	A	194	ALA
1	A	319	GLY
1	A	385	ILE
1	A	418	SER
1	A	567	LYS
1	A	629	LEU
1	A	640	GLN
1	A	751	SER
1	A	775	ILE
1	A	1016	THR
1	A	1064	VAL
1	A	1092	LYS
1	A	1108	ALA
2	B	58	THR
2	B	80	GLU
2	B	137	TYR
2	B	146	GLU
2	B	148	LYS
2	B	161	GLU
2	B	221	ASN
2	B	282	ILE
2	B	334	ILE
2	B	345	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	440	HIS
2	B	507	LYS
2	B	712	PRO
2	B	907	GLY
2	B	921	ASP
2	B	1157	ALA
3	C	142	VAL
3	C	161	LYS
4	D	19	GLU
4	D	20	GLU
4	D	199	ASN
5	E	115	ASN
5	E	172	GLU
6	F	73	ALA
7	G	141	SER
7	G	153	GLN
10	J	2	ILE
1	A	5	GLN
1	A	59	GLY
1	A	131	SER
1	A	156	ASP
1	A	286	HIS
1	A	628	GLY
1	A	1085	HIS
1	A	1112	LYS
1	A	1221	LYS
1	A	1403	GLU
1	A	1437	GLY
2	B	81	SER
2	B	199	MET
2	B	247	GLY
2	B	252	SER
2	B	470	LYS
2	B	511	PRO
2	B	575	PRO
2	B	648	HIS
2	B	926	GLY
2	B	931	TYR
2	B	933	SER
2	B	935	ARG
2	B	943	SER
3	C	91	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	215	GLU
4	D	15	LEU
4	D	169	SER
5	E	45	LYS
8	H	109	LYS
8	H	129	TYR
9	I	106	CYS
12	L	45	ALA
1	A	4	GLN
1	A	146	MET
1	A	465	TYR
1	A	593	GLU
1	A	1081	LEU
1	A	1206	ASP
1	A	1270	ASN
1	A	1404	GLU
2	B	78	THR
2	B	249	ARG
2	B	250	PHE
2	B	347	LYS
2	B	441	ASP
2	B	531	GLN
2	B	711	GLU
2	B	869	SER
2	B	889	THR
4	D	8	PHE
4	D	16	LYS
4	D	118	THR
4	D	198	LEU
5	E	3	GLN
5	E	50	MET
7	G	50	ASP
8	H	17	PRO
8	H	60	ALA
8	H	108	SER
9	I	11	ASN
12	L	59	ALA
1	A	42	ASP
1	A	67	CYS
1	A	595	THR
1	A	1107	VAL
2	B	465	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	831	SER
2	B	832	GLY
2	B	884	ARG
2	B	951	GLN
2	B	1041	GLU
2	B	1181	GLU
3	C	90	ASP
3	C	174	ALA
6	F	72	LYS
7	G	132	SER
7	G	154	VAL
8	H	78	SER
11	K	70	ARG
12	L	41	SER
1	A	54	ASN
1	A	152	VAL
1	A	158	PRO
1	A	188	ASP
1	A	399	HIS
1	A	423	ASP
1	A	424	ILE
1	A	453	MET
1	A	626	ASN
1	A	779	PHE
1	A	958	VAL
1	A	1086	PHE
1	A	1094	VAL
1	A	1111	MET
1	A	1120	LEU
1	A	1314	SER
2	B	608	ASP
2	B	922	GLU
2	B	961	LEU
2	B	1046	PRO
5	E	104	ASN
7	G	63	PRO
8	H	128	ASN
9	I	21	GLU
1	A	568	PRO
1	A	1115	SER
2	B	751	VAL
2	B	1045	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	175	ALA
4	D	11	ARG
1	A	61	ILE
1	A	410	GLY
1	A	147	VAL
1	A	308	ILE
5	E	127	ILE
2	B	143	PRO
2	B	343	ILE
8	H	85	GLY

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	1250/1520 (82%)	1148 (92%)	102 (8%)	10	34
2	B	1009/1061 (95%)	938 (93%)	71 (7%)	14	38
3	C	233/274 (85%)	215 (92%)	18 (8%)	12	35
4	D	156/200 (78%)	147 (94%)	9 (6%)	18	42
5	E	196/197 (100%)	187 (95%)	9 (5%)	24	47
6	F	77/137 (56%)	72 (94%)	5 (6%)	15	40
7	G	152/160 (95%)	139 (91%)	13 (9%)	10	33
8	H	118/128 (92%)	113 (96%)	5 (4%)	26	49
9	I	107/116 (92%)	105 (98%)	2 (2%)	50	67
10	J	61/65 (94%)	54 (88%)	7 (12%)	5	22
11	K	99/102 (97%)	92 (93%)	7 (7%)	13	38
12	L	39/57 (68%)	31 (80%)	8 (20%)	1	8
All	All	3497/4017 (87%)	3241 (93%)	256 (7%)	13	37

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	35	ILE
1	A	43	GLU
1	A	44	THR
1	A	50	ILE
1	A	61	ILE
1	A	77	CYS
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL
1	A	117	GLU
1	A	128	ILE
1	A	129	LYS
1	A	141	LEU
1	A	152	VAL
1	A	187	LYS
1	A	204	THR
1	A	226	GLU
1	A	247	ARG
1	A	256	GLN
1	A	270	LEU
1	A	276	LEU
1	A	329	LEU
1	A	337	ARG
1	A	375	THR
1	A	385	ILE
1	A	419	LYS
1	A	433	GLU
1	A	443	LEU
1	A	447	GLN
1	A	468	PHE
1	A	470	LEU
1	A	475	THR
1	A	487	MET
1	A	505	CYS
1	A	509	LEU
1	A	511	ILE
1	A	513	SER
1	A	518	LYS
1	A	524	VAL
1	A	527	THR
1	A	567	LYS
1	A	595	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	597	LEU
1	A	636	GLU
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	701	LEU
1	A	702	LEU
1	A	771	GLU
1	A	774	ARG
1	A	821	ARG
1	A	825	ILE
1	A	837	ILE
1	A	838	GLN
1	A	840	ARG
1	A	860	LEU
1	A	878	ILE
1	A	899	VAL
1	A	919	ILE
1	A	932	GLU
1	A	973	ILE
1	A	980	ASP
1	A	981	LEU
1	A	983	ILE
1	A	1003	LYS
1	A	1016	THR
1	A	1021	LEU
1	A	1022	LEU
1	A	1032	LEU
1	A	1037	LEU
1	A	1077	THR
1	A	1080	THR
1	A	1081	LEU
1	A	1086	PHE
1	A	1101	LEU
1	A	1107	VAL
1	A	1110	ASN
1	A	1116	LEU
1	A	1120	LEU
1	A	1134	ILE
1	A	1135	ARG
1	A	1143	LEU
1	A	1215	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1238	ILE
1	A	1286	LYS
1	A	1289	ARG
1	A	1303	GLU
1	A	1306	LEU
1	A	1315	GLU
1	A	1316	VAL
1	A	1345	ARG
1	A	1356	ILE
1	A	1366	ARG
1	A	1371	LEU
1	A	1394	THR
1	A	1404	GLU
1	A	1409	LEU
1	A	1411	GLU
1	A	1436	ILE
1	A	1447	GLU
2	B	28	GLU
2	B	47	GLN
2	B	63	ILE
2	B	65	GLU
2	B	84	ILE
2	B	167	ILE
2	B	175	ARG
2	B	178	ASN
2	B	217	ARG
2	B	221	ASN
2	B	228	LYS
2	B	240	ILE
2	B	251	ILE
2	B	269	ILE
2	B	282	ILE
2	B	309	GLN
2	B	324	ILE
2	B	341	LEU
2	B	364	ILE
2	B	401	PHE
2	B	424	LEU
2	B	431	TYR
2	B	497	ARG
2	B	505	ASP
2	B	526	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	529	GLU
2	B	555	ILE
2	B	570	VAL
2	B	585	VAL
2	B	612	GLU
2	B	633	VAL
2	B	658	ILE
2	B	698	GLU
2	B	711	GLU
2	B	748	ILE
2	B	783	THR
2	B	795	ILE
2	B	797	TYR
2	B	807	ARG
2	B	822	ASN
2	B	825	VAL
2	B	829	CYS
2	B	836	GLU
2	B	837	ASP
2	B	841	MET
2	B	865	LYS
2	B	874	PHE
2	B	921	ASP
2	B	944	THR
2	B	945	GLU
2	B	972	LYS
2	B	973	ILE
2	B	986	GLN
2	B	987	LYS
2	B	1011	ILE
2	B	1055	ILE
2	B	1072	MET
2	B	1093	GLN
2	B	1108	ARG
2	B	1117	GLN
2	B	1123	SER
2	B	1150	ARG
2	B	1159	ARG
2	B	1162	ILE
2	B	1166	CYS
2	B	1176	ASN
2	B	1183	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1194	ILE
2	B	1202	LEU
2	B	1217	TYR
2	B	1220	ARG
3	C	27	LEU
3	C	55	THR
3	C	56	THR
3	C	77	ILE
3	C	94	LYS
3	C	100	THR
3	C	101	LEU
3	C	133	ILE
3	C	137	LYS
3	C	147	LEU
3	C	179	GLU
3	C	186	LEU
3	C	197	SER
3	C	203	GLN
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	251	LEU
4	D	50	LEU
4	D	51	ASN
4	D	120	GLU
4	D	124	GLU
4	D	131	GLU
4	D	144	THR
4	D	145	MET
4	D	152	SER
4	D	214	LEU
5	E	69	ILE
5	E	81	GLU
5	E	121	MET
5	E	132	ILE
5	E	170	LEU
5	E	175	LEU
5	E	191	LYS
5	E	198	ILE
5	E	207	ARG
6	F	72	LYS
6	F	74	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	77	ASP
6	F	112	GLU
6	F	123	LYS
7	G	6	ASP
7	G	13	LEU
7	G	31	LEU
7	G	39	THR
7	G	46	LEU
7	G	112	LYS
7	G	115	MET
7	G	133	SER
7	G	134	GLU
7	G	143	ILE
7	G	154	VAL
7	G	160	ILE
7	G	171	ILE
8	H	26	ILE
8	H	40	LEU
8	H	46	LEU
8	H	63	LEU
8	H	135	LEU
9	I	26	LEU
9	I	87	GLN
10	J	2	ILE
10	J	3	VAL
10	J	9	SER
10	J	22	LEU
10	J	24	LEU
10	J	38	ARG
10	J	46	CYS
11	K	12	LEU
11	K	42	LEU
11	K	49	GLU
11	K	73	LEU
11	K	75	ILE
11	K	102	LYS
11	K	114	LEU
12	L	27	LEU
12	L	33	GLU
12	L	40	LEU
12	L	42	ARG
12	L	43	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	54	ARG
12	L	56	LEU
12	L	58	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	68	GLN
1	A	525	GLN
1	A	626	ASN
1	A	648	ASN
1	A	717	ASN
1	A	736	ASN
1	A	767	GLN
1	A	811	GLN
1	A	854	ASN
1	A	877	HIS
1	A	881	GLN
1	A	1128	GLN
1	A	1187	GLN
1	A	1265	ASN
1	A	1390	ASN
2	B	77	HIS
2	B	121	ASN
2	B	215	GLN
2	B	224	GLN
2	B	255	GLN
2	B	325	GLN
2	B	357	GLN
2	B	494	HIS
2	B	572	HIS
2	B	592	ASN
2	B	767	ASN
2	B	862	GLN
2	B	1062	HIS
2	B	1084	GLN
2	B	1093	GLN
2	B	1179	GLN
2	B	1193	GLN
2	B	1205	GLN
2	B	1211	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	7	GLN
3	C	73	GLN
3	C	123	ASN
3	C	231	ASN
4	D	9	GLN
4	D	51	ASN
4	D	132	GLN
4	D	199	ASN
5	E	5	ASN
5	E	106	GLN
7	G	53	ASN
7	G	96	GLN
7	G	97	HIS
7	G	126	ASN
7	G	153	GLN
7	G	158	HIS
8	H	11	GLN
8	H	33	GLN
9	I	46	HIS
9	I	51	ASN
9	I	83	ASN
9	I	108	HIS
11	K	29	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	7/9 (77%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 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, 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	1436/1733 (82%)	0.08	13 (0%) 81 64	62, 176, 266, 296	0
2	B	1172/1224 (95%)	0.19	23 (1%) 65 48	73, 189, 282, 300	0
3	C	265/318 (83%)	0.06	0 100 100	95, 184, 251, 288	0
4	D	178/221 (80%)	-0.02	2 (1%) 78 60	128, 206, 266, 293	0
5	E	214/215 (99%)	0.13	1 (0%) 87 73	105, 228, 280, 291	0
6	F	87/155 (56%)	-0.08	1 (1%) 78 60	86, 151, 218, 234	0
7	G	171/179 (95%)	0.04	3 (1%) 67 50	120, 178, 253, 300	0
8	H	135/146 (92%)	0.14	3 (2%) 62 46	158, 232, 286, 294	0
9	I	114/122 (93%)	0.22	2 (1%) 67 50	137, 224, 283, 293	0
10	J	66/70 (94%)	0.22	3 (4%) 38 30	92, 186, 243, 270	0
11	K	115/120 (95%)	0.01	0 100 100	92, 175, 245, 284	0
12	L	44/70 (62%)	0.35	1 (2%) 61 45	142, 237, 271, 297	0
13	R	9/9 (100%)	-0.30	0 100 100	201, 226, 298, 299	0
14	S	38/53 (71%)	0.75	1 (2%) 57 42	300, 300, 300, 300	0
15	U	40/53 (75%)	0.79	2 (5%) 34 28	183, 300, 300, 300	0
All	All	4084/4688 (87%)	0.12	55 (1%) 75 57	62, 189, 282, 300	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	6	SER	4.6
1	A	79	GLY	3.8
2	B	486	TYR	3.5
1	A	114	LEU	3.4
1	A	2	VAL	3.2
2	B	1009	ASP	3.2
2	B	531	GLN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	3.0
7	G	51	TYR	2.9
8	H	61	SER	2.8
9	I	64	SER	2.8
2	B	283	VAL	2.8
2	B	742	GLU	2.8
5	E	90	VAL	2.7
1	A	1407	GLU	2.7
1	A	664	THR	2.6
2	B	710	LEU	2.6
2	B	1107	ALA	2.5
1	A	811	GLN	2.5
2	B	502	ILE	2.5
8	H	119	GLY	2.5
10	J	15	GLY	2.5
2	B	268	THR	2.5
2	B	916	THR	2.5
2	B	930	ALA	2.5
2	B	1096	ARG	2.4
1	A	596	THR	2.4
2	B	252	SER	2.4
1	A	1395	GLY	2.4
2	B	1167	GLY	2.4
7	G	127	PRO	2.3
2	B	253	THR	2.3
12	L	55	ILE	2.3
1	A	34	LYS	2.3
2	B	925	LEU	2.3
2	B	509	ALA	2.3
2	B	193	LYS	2.1
15	U	28	DA	2.1
10	J	66	LEU	2.1
2	B	736	THR	2.1
2	B	1173	ALA	2.1
1	A	1352	VAL	2.1
4	D	170	THR	2.1
6	F	143	PHE	2.1
1	A	990	VAL	2.1
2	B	954	VAL	2.1
1	A	1001	ARG	2.0
14	S	12	DA	2.0
15	U	27	DA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	76	THR	2.0
2	B	529	GLU	2.0
7	G	113	HIS	2.0
9	I	69	PRO	2.0
2	B	266	ALA	2.0
10	J	16	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	MG	A	1804	1/1	0.58	0.31	166,166,166,166	0
17	MG	A	1803	1/1	0.74	0.33	171,171,171,171	0
16	ZN	C	401	1/1	0.91	0.14	174,174,174,174	0
16	ZN	B	1301	1/1	0.98	0.08	166,166,166,166	0
16	ZN	L	101	1/1	0.98	0.06	188,188,188,188	0
16	ZN	A	1802	1/1	0.99	0.04	166,166,166,166	0
16	ZN	I	201	1/1	0.99	0.06	173,173,173,173	0
16	ZN	I	202	1/1	0.99	0.05	216,216,216,216	0
16	ZN	A	1801	1/1	1.00	0.02	153,153,153,153	0
16	ZN	C	402	1/1	1.00	0.03	148,148,148,148	0
16	ZN	J	101	1/1	1.00	0.06	172,172,172,172	0

6.5 Other polymers [i](#)

There are no such residues in this entry.