



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:17 PM GMT

PDB ID : 1NGM
Title : Crystal structure of a yeast Brf1-TBP-DNA ternary complex
Authors : Juo, Z.S.; Kassavetis, G.A.; Wang, J.; Geiduschek, E.P.; Sigler, P.B.
Deposited on : 2002-12-17
Resolution : 2.95 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

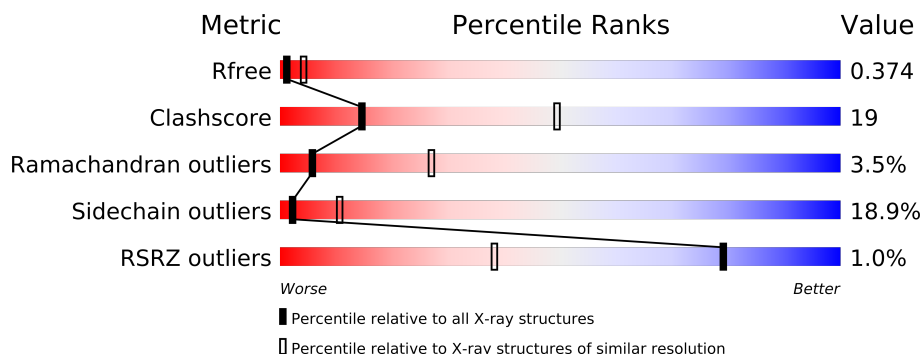
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.95 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.



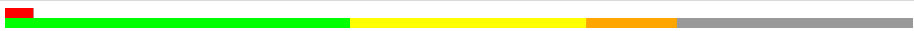

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	19	
1	G	19	
1	K	19	
1	O	19	
2	D	19	
2	H	19	
2	L	19	
2	P	19	
3	A	180	
3	E	180	
3	I	180	
3	M	180	
4	B	72	
4	F	72	

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Mol	Chain	Length	Quality of chain
4	J	72	
4	N	72	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10800 atoms, of which 0 are hydrogen and 0 are deuterium.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	19	Total	C	N	O	P	0	0	0
			386	189	66	113	18			
1	G	19	Total	C	N	O	P	0	0	0
			386	189	66	113	18			
1	K	19	Total	C	N	O	P	0	0	0
			386	189	66	113	18			
1	O	19	Total	C	N	O	P	0	0	0
			386	189	66	113	18			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*AP*AP*AP*AP*CP*AP*TP*TP*TP*TP
*TP*TP*TP*AP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	P	0	0	0
			387	189	69	111	18			
2	H	19	Total	C	N	O	P	0	0	0
			387	189	69	111	18			
2	L	19	Total	C	N	O	P	0	0	0
			387	189	69	111	18			
2	P	19	Total	C	N	O	P	0	0	0
			387	189	69	111	18			

- Molecule 3 is a protein called Transcription initiation factor TFIID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	180	Total	C	N	O	S	0	0	0
			1416	921	242	247	6			
3	E	180	Total	C	N	O	S	0	0	0
			1416	921	242	247	6			
3	I	180	Total	C	N	O	S	0	0	0
			1416	921	242	247	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	180	Total	C	N	O	S	0	0	0
			1416	921	242	247	6			

- Molecule 4 is a protein called Transcription factor IIIB BRF1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	72	Total	C	N	O	S	0	0	0
			586	363	98	124	1			
4	F	72	Total	C	N	O	S	0	0	0
			586	363	98	124	1			
4	J	53	Total	C	N	O		0	0	0
			436	268	73	95				
4	N	53	Total	C	N	O		0	0	0
			436	268	73	95				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	435	GLY	-	CLONING ARTIFACT	UNP P29056
B	436	SER	-	CLONING ARTIFACT	UNP P29056
F	435	GLY	-	CLONING ARTIFACT	UNP P29056
F	436	SER	-	CLONING ARTIFACT	UNP P29056
J	435	GLY	-	CLONING ARTIFACT	UNP P29056
J	436	SER	-	CLONING ARTIFACT	UNP P29056
N	435	GLY	-	CLONING ARTIFACT	UNP P29056
N	436	SER	-	CLONING ARTIFACT	UNP P29056

Chain H: 



- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*AP*CP*AP*TP*TP*TP*TP*TP*TP*TP*TP*AP*TP*A P*G)-3'

Chain L: 



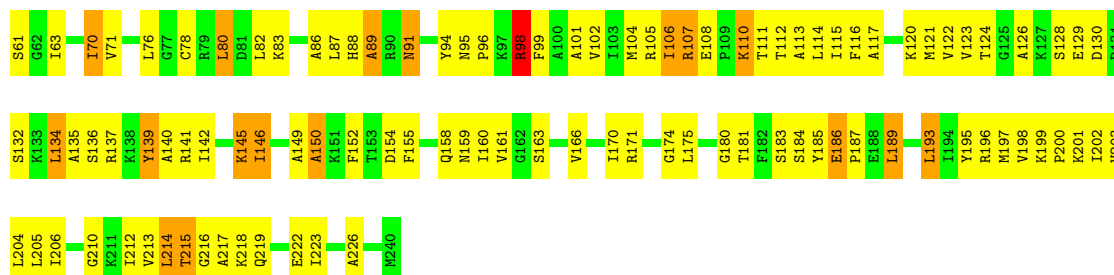
- Molecule 2: 5'-D(*AP*AP*AP*AP*AP*AP*CP*AP*TP*TP*TP*TP*TP*TP*TP*TP*AP*TP*A P*G)-3'

Chain P: 



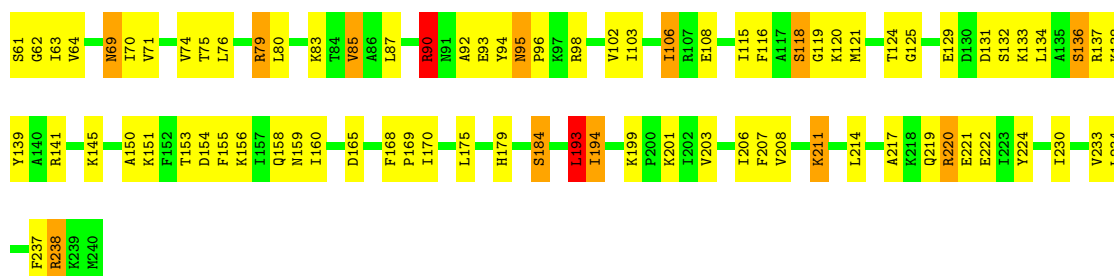
- Molecule 3: Transcription initiation factor TFIID

Chain A: 



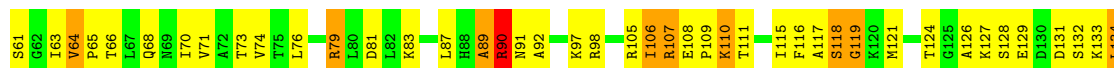
- Molecule 3: Transcription initiation factor TFIID

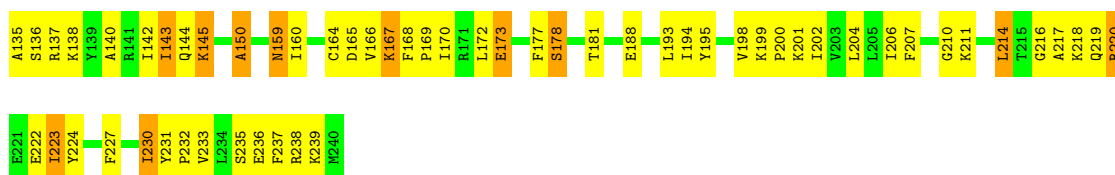
Chain E: 



- Molecule 3: Transcription initiation factor TFIID

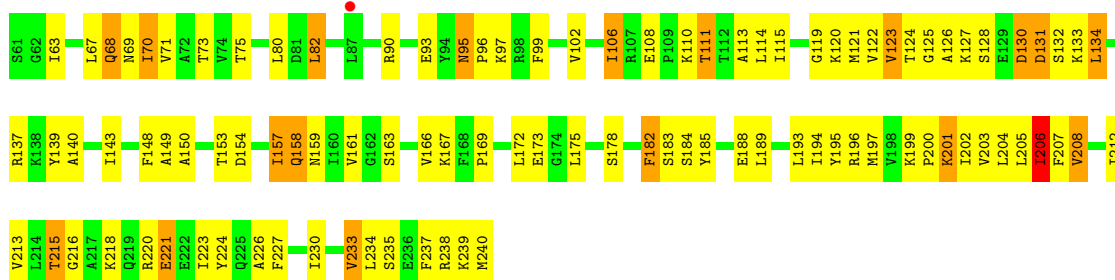
Chain I: 





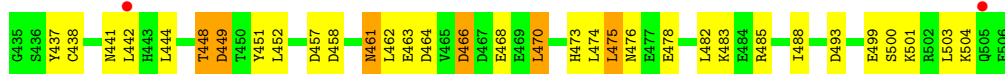
- Molecule 3: Transcription initiation factor TFIID

Chain M:



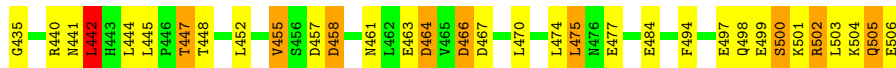
- Molecule 4: Transcription factor IIIB BRF1 subunit

Chain B:



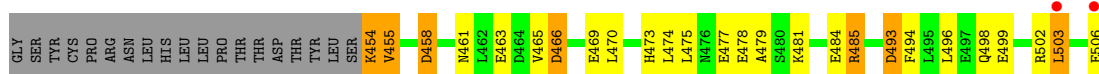
- Molecule 4: Transcription factor IIIB BRF1 subunit

Chain F:



- Molecule 4: Transcription factor IIIB BRF1 subunit

Chain J:



- Molecule 4: Transcription factor IIIB BRF1 subunit

Chain N:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.61Å 152.60Å 256.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 47.29 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.95) 95.2 (47.29-2.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.276 , 0.308 0.365 , 0.374	Depositor DCC
R_{free} test set	7533 reflections (10.09%)	DCC
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 1.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Outliers	0 of 74659 reflections	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	10800	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.18 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.0154e-03.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.79	0/432	1.52	2/665 (0.3%)
1	G	1.03	2/432 (0.5%)	1.80	12/665 (1.8%)
1	K	0.98	0/432	1.80	15/665 (2.3%)
1	O	0.83	0/432	1.72	10/665 (1.5%)
2	D	0.77	0/434	1.59	9/668 (1.3%)
2	H	0.86	0/434	1.62	9/668 (1.3%)
2	L	1.01	0/434	1.81	14/668 (2.1%)
2	P	0.82	0/434	1.47	6/668 (0.9%)
3	A	0.41	0/1443	0.68	1/1942 (0.1%)
3	E	0.59	0/1443	0.82	2/1942 (0.1%)
3	I	0.59	0/1443	0.83	2/1942 (0.1%)
3	M	0.43	0/1443	0.70	2/1942 (0.1%)
4	B	0.35	0/595	0.82	5/804 (0.6%)
4	F	0.54	0/595	0.91	4/804 (0.5%)
4	J	0.48	0/440	0.85	2/590 (0.3%)
4	N	0.31	0/440	0.80	5/590 (0.8%)
All	All	0.64	2/11306 (0.0%)	1.16	100/15888 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	5	DA	C3'-O3'	-5.62	1.36	1.44
1	G	9	DA	C3'-O3'	-5.05	1.37	1.44

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	16	DA	O4'-C1'-N9	12.42	116.69	108.00
1	K	6	DA	O4'-C1'-N9	11.14	115.80	108.00
1	O	1	DC	O4'-C1'-N1	10.36	115.25	108.00
1	G	2	DT	O4'-C4'-C3'	-10.09	99.94	106.00
2	D	5	DA	O4'-C1'-N9	9.88	114.91	108.00
1	C	10	DA	O4'-C1'-N9	9.18	114.42	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7	DC	O4'-C1'-N1	9.14	114.40	108.00
1	G	7	DA	O4'-C1'-N9	9.09	114.36	108.00
1	O	15	DT	O4'-C1'-N1	8.27	113.79	108.00
1	O	8	DA	O4'-C4'-C3'	-8.06	101.16	106.00
1	O	11	DA	O4'-C1'-N9	7.76	113.43	108.00
1	G	5	DA	O4'-C4'-C3'	7.69	110.61	106.00
2	L	15	DT	O4'-C1'-N1	-7.29	102.90	108.00
2	P	13	DT	O4'-C4'-C3'	-7.16	101.64	104.50
3	E	193	LEU	CA-CB-CG	7.08	131.59	115.30
1	O	15	DT	C1'-O4'-C4'	-7.06	103.04	110.10
1	K	16	DT	O4'-C1'-N1	6.97	112.88	108.00
2	L	17	DT	C5-C4-O4	-6.96	120.03	124.90
1	G	4	DT	C4-C5-C7	6.92	123.15	119.00
2	P	15	DT	O4'-C1'-N1	6.77	112.74	108.00
4	N	467	ASP	CB-CG-OD2	6.76	124.38	118.30
1	G	4	DT	C6-C5-C7	-6.75	118.85	122.90
2	H	19	DG	O4'-C4'-C3'	-6.71	101.81	104.50
1	G	5	DA	O4'-C1'-N9	6.61	112.62	108.00
3	M	130	ASP	CB-CG-OD2	6.60	124.24	118.30
1	K	4	DT	C6-C5-C7	-6.56	118.96	122.90
2	H	14	DT	C5-C4-O4	-6.50	120.35	124.90
2	L	12	DT	C6-C5-C7	-6.50	119.00	122.90
2	D	5	DA	C1'-O4'-C4'	-6.44	103.66	110.10
1	O	15	DT	O4'-C1'-C2'	-6.39	100.79	105.90
1	O	5	DA	O4'-C1'-N9	6.34	112.44	108.00
2	L	12	DT	C4-C5-C7	6.32	122.79	119.00
2	L	17	DT	N3-C4-O4	6.30	123.68	119.90
2	H	14	DT	N3-C4-O4	6.25	123.65	119.90
3	I	131	ASP	CB-CG-OD2	6.17	123.86	118.30
1	K	1	DC	O4'-C1'-N1	-6.17	103.68	108.00
2	L	9	DT	P-O3'-C3'	6.15	127.08	119.70
2	P	12	DT	O4'-C1'-N1	6.12	112.28	108.00
2	P	8	DA	P-O3'-C3'	6.10	127.03	119.70
2	D	1	DA	O4'-C1'-N9	6.10	112.27	108.00
1	K	6	DA	O4'-C4'-C3'	6.09	109.66	106.00
1	G	2	DT	C5-C4-O4	-6.06	120.66	124.90
2	L	19	DG	O4'-C1'-N9	-6.06	103.76	108.00
1	O	13	DG	O4'-C1'-N9	6.05	112.24	108.00
1	K	2	DT	O4'-C4'-C3'	-6.01	102.09	104.50
1	O	7	DA	O4'-C1'-N9	6.00	112.20	108.00
2	D	12	DT	C4-C5-C7	5.99	122.60	119.00
4	B	449	ASP	CB-CG-OD2	5.97	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	DA	O4'-C1'-N9	5.96	112.17	108.00
1	K	4	DT	C4-C5-C7	5.96	122.58	119.00
2	L	18	DA	O5'-P-OP1	-5.93	100.36	105.70
1	K	3	DA	C2-N3-C4	5.91	113.55	110.60
3	I	81	ASP	CB-CG-OD2	5.91	123.62	118.30
2	D	18	DA	C1'-O4'-C4'	-5.90	104.20	110.10
2	L	9	DT	O4'-C1'-N1	-5.88	103.88	108.00
4	F	464	ASP	CB-CG-OD2	5.87	123.58	118.30
2	D	11	DT	O4'-C1'-N1	5.77	112.04	108.00
1	G	2	DT	N3-C4-O4	5.77	123.36	119.90
1	O	9	DA	O4'-C1'-N9	5.69	111.98	108.00
1	G	17	DT	O4'-C1'-N1	5.66	111.96	108.00
4	F	458	ASP	CB-CG-OD2	5.64	123.37	118.30
2	D	7	DC	O4'-C1'-N1	5.63	111.94	108.00
4	F	457	ASP	CB-CG-OD2	5.62	123.36	118.30
2	P	14	DT	N3-C4-O4	5.58	123.25	119.90
4	N	460	ASP	CB-CG-OD2	5.54	123.29	118.30
2	L	18	DA	O4'-C1'-N9	5.53	111.87	108.00
1	K	9	DA	O4'-C1'-N9	5.50	111.85	108.00
2	D	12	DT	C6-C5-C7	-5.41	119.65	122.90
4	J	458	ASP	CB-CG-OD2	5.36	123.13	118.30
2	H	17	DT	O4'-C4'-C3'	-5.35	102.36	104.50
2	H	9	DT	N3-C4-O4	5.35	123.11	119.90
3	A	80	LEU	CA-CB-CG	5.35	127.59	115.30
1	K	16	DT	O4'-C1'-C2'	-5.34	101.63	105.90
4	N	493	ASP	CB-CG-OD2	5.32	123.08	118.30
2	P	17	DT	N3-C4-O4	5.31	123.08	119.90
1	G	5	DA	O4'-C1'-C2'	5.27	110.11	105.90
4	B	493	ASP	CB-CG-OD2	5.25	123.03	118.30
2	H	16	DA	OP2-P-O3'	5.23	116.70	105.20
4	J	493	ASP	CB-CG-OD2	5.22	123.00	118.30
2	H	14	DT	O4'-C1'-C2'	5.19	110.05	105.90
1	K	2	DT	N3-C2-O2	-5.17	119.20	122.30
1	K	15	DT	O4'-C1'-C2'	-5.14	101.79	105.90
1	K	14	DT	C3'-C2'-C1'	-5.13	96.34	102.50
3	M	154	ASP	CB-CG-OD2	5.12	122.91	118.30
1	G	6	DA	N1-C6-N6	5.11	121.67	118.60
1	G	13	DG	O4'-C1'-N9	5.09	111.56	108.00
2	L	14	DT	P-O5'-C5'	-5.08	112.77	120.90
4	B	466	ASP	CB-CG-OD2	5.07	122.86	118.30
4	N	458	ASP	CB-CG-OD2	5.07	122.86	118.30
2	D	18	DA	C3'-C2'-C1'	-5.05	96.44	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	458	ASP	CB-CG-OD2	5.05	122.84	118.30
4	B	457	ASP	CB-CG-OD2	5.05	122.84	118.30
4	N	464	ASP	CB-CG-OD2	5.04	122.84	118.30
1	K	17	DT	O4'-C1'-N1	5.04	111.53	108.00
2	L	17	DT	P-O5'-C5'	-5.04	112.84	120.90
1	K	18	DT	O4'-C1'-N1	5.03	111.52	108.00
3	E	131	ASP	CB-CG-OD2	5.02	122.82	118.30
2	L	16	DA	O4'-C4'-C3'	5.02	109.01	106.00
4	F	466	ASP	CB-CG-OD2	5.02	122.82	118.30
2	H	17	DT	C1'-O4'-C4'	-5.01	105.09	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	386	0	220	14	0
1	G	386	0	220	9	0
1	K	386	0	220	5	0
1	O	386	0	220	20	0
2	D	387	0	219	9	0
2	H	387	0	219	15	0
2	L	387	0	219	12	0
2	P	387	0	219	17	0
3	A	1416	0	1493	86	0
3	E	1416	0	1493	64	0
3	I	1416	0	1493	79	0
3	M	1416	0	1493	74	0
4	B	586	0	562	23	0
4	F	586	0	562	30	0
4	J	436	0	417	17	0
4	N	436	0	417	5	0
All	All	10800	0	9686	394	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (394) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:111:THR:HG21	3:A:135:ALA:HB1	1.25	1.19
2:L:13:DT:H2"	2:L:14:DT:H5"	1.23	1.12
3:A:111:THR:HG21	3:A:135:ALA:CB	1.82	1.08
3:I:89:ALA:O	4:J:475:LEU:HG	1.62	0.99
3:I:145:LYS:HG2	4:J:474:LEU:HD11	1.45	0.98
1:G:5:DA:H5"	3:E:203:VAL:HG21	1.42	0.98
3:E:129:GLU:HG2	4:F:448:THR:HG23	1.47	0.95
3:E:90:ARG:HH11	3:E:90:ARG:HG2	1.32	0.93
3:A:129:GLU:HB2	4:B:451:TYR:HB3	1.50	0.90
3:E:79:ARG:HA	3:E:118:SER:O	1.73	0.88
3:E:156:LYS:HE3	3:E:158:GLN:HE22	1.41	0.85
4:F:435:GLY:HA2	3:I:128:SER:HB3	1.58	0.84
3:A:71:VAL:HG22	3:A:124:THR:HG22	1.64	0.79
3:M:169:PRO:HB2	3:M:239:LYS:HB3	1.65	0.79
2:L:14:DT:OP1	3:I:105:ARG:NH1	2.16	0.78
3:A:214:LEU:HD21	3:A:226:ALA:HB3	1.64	0.78
3:A:89:ALA:HA	4:B:473:HIS:O	1.82	0.78
2:L:13:DT:H2"	2:L:14:DT:C5'	2.08	0.78
3:A:115:ILE:HD12	3:A:121:MET:HB3	1.67	0.76
3:E:90:ARG:HG2	3:E:90:ARG:NH1	1.98	0.76
3:E:237:PHE:O	3:E:238:ARG:CB	2.33	0.76
3:M:82:LEU:HG	3:M:102:VAL:HG23	1.66	0.75
3:A:106:ILE:HG13	3:A:107:ARG:N	2.00	0.75
3:I:168:PHE:CD1	3:I:238:ARG:HG3	2.22	0.74
1:C:9:DA:H1'	1:C:10:DA:C8	2.23	0.73
3:A:102:VAL:HB	3:A:115:ILE:HG22	1.71	0.73
3:A:202:ILE:HG12	3:A:217:ALA:HB2	1.72	0.71
3:E:64:VAL:HG11	3:I:64:VAL:HG22	1.73	0.71
3:I:204:LEU:HD21	3:I:230:ILE:HG21	1.72	0.71
3:I:74:VAL:HG11	3:I:121:MET:HE3	1.73	0.70
3:M:184:SER:HB2	3:M:194:ILE:HB	1.72	0.70
3:M:182:PHE:N	3:M:182:PHE:HD1	1.89	0.70
3:E:156:LYS:HE3	3:E:158:GLN:NE2	2.07	0.70
3:I:79:ARG:HA	3:I:118:SER:O	1.91	0.70
4:J:485:ARG:HG3	4:J:485:ARG:HH11	1.57	0.70
2:P:16:DA:C2	3:M:213:VAL:HG11	2.28	0.69
3:M:206:ILE:HD13	3:M:212:ILE:HD12	1.73	0.69
3:A:111:THR:CG2	3:A:135:ALA:HB1	2.15	0.69
3:E:237:PHE:O	3:E:238:ARG:HB3	1.92	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:182:PHE:CD1	3:M:182:PHE:N	2.60	0.68
3:M:71:VAL:HB	3:M:159:ASN:HB3	1.76	0.68
4:B:466:ASP:HA	4:B:470:LEU:HD22	1.76	0.68
3:M:68:GLN:HG3	3:M:163:SER:HB3	1.75	0.67
3:M:133:LYS:HD2	4:N:455:VAL:CG1	2.24	0.67
3:M:99:PHE:HE2	3:M:114:LEU:HD22	1.59	0.67
3:M:183:SER:HB3	3:M:193:LEU:HD21	1.77	0.67
3:A:111:THR:CG2	3:A:135:ALA:CB	2.69	0.66
2:D:1:DA:H2''	2:D:2:DA:H5'	1.78	0.66
1:O:4:DT:H3	2:P:16:DA:H61	1.43	0.66
3:A:82:LEU:HG	3:A:117:ALA:HB2	1.78	0.66
3:A:113:ALA:HA	3:A:123:VAL:HA	1.78	0.65
3:M:195:TYR:HB3	3:M:204:LEU:HB2	1.77	0.65
3:E:95:ASN:C	3:E:95:ASN:HD22	2.00	0.65
3:M:69:ASN:HD21	3:M:125:GLY:H	1.41	0.65
3:M:207:PHE:HE2	3:M:213:VAL:HG23	1.62	0.65
3:M:128:SER:HB3	3:M:131:ASP:HB2	1.80	0.64
3:I:173:GLU:CD	3:I:173:GLU:H	2.00	0.64
1:C:19:DT:H2'	2:H:1:DA:C2	2.33	0.64
2:H:1:DA:H2'	2:H:2:DA:C8	2.32	0.64
3:E:90:ARG:CG	3:E:90:ARG:HH11	2.10	0.63
2:P:16:DA:H2	3:M:213:VAL:HG11	1.63	0.63
3:A:214:LEU:HD21	3:A:226:ALA:CB	2.27	0.63
1:O:6:DA:H2	3:M:71:VAL:HG21	1.63	0.63
1:G:5:DA:C5'	3:E:203:VAL:HG21	2.25	0.63
3:E:90:ARG:HA	4:F:475:LEU:HD21	1.81	0.63
1:G:17:DT:H2'	1:G:18:DT:C6	2.33	0.62
2:H:17:DT:H5''	3:E:211:LYS:HZ2	1.64	0.62
3:M:172:LEU:HG	3:M:208:VAL:HG13	1.79	0.62
4:F:435:GLY:HA2	3:I:128:SER:CB	2.28	0.62
3:A:142:ILE:O	3:A:146:ILE:HG13	2.00	0.62
3:I:76:LEU:HB2	3:I:119:GLY:O	2.00	0.61
3:A:111:THR:HG21	3:A:135:ALA:HB2	1.77	0.61
1:O:4:DT:H2''	1:O:5:DA:H5'	1.82	0.61
3:I:164:CYS:SG	3:I:227:PHE:CE1	2.95	0.60
3:A:91:ASN:HB2	3:A:104:MET:HA	1.83	0.60
4:F:440:ARG:HH11	4:F:440:ARG:HG3	1.65	0.60
3:A:129:GLU:HB2	4:B:451:TYR:CB	2.27	0.60
4:F:448:THR:HG22	4:F:452:LEU:CD1	2.30	0.60
3:E:76:LEU:HA	3:E:151:LYS:O	2.02	0.60
4:J:485:ARG:HG3	4:J:485:ARG:NH1	2.16	0.60
3:I:74:VAL:HG11	3:I:121:MET:CE	2.32	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:3:DA:H2''	1:O:4:DT:H5'	1.83	0.59
3:E:83:LYS:O	3:E:87:LEU:HG	2.02	0.59
3:E:137:ARG:NH1	4:F:464:ASP:OD1	2.36	0.59
3:I:71:VAL:HG22	3:I:124:THR:HG22	1.84	0.59
1:O:7:DA:H2''	1:O:8:DA:O4'	2.03	0.59
4:F:440:ARG:HD3	4:F:445:LEU:HD11	1.85	0.59
2:D:12:DT:H5''	3:A:98:ARG:HD3	1.84	0.59
2:H:17:DT:H5''	3:E:211:LYS:NZ	2.18	0.59
1:C:7:DA:H2''	1:C:8:DA:H5'	1.84	0.58
3:M:133:LYS:HD2	4:N:455:VAL:HG11	1.85	0.58
1:C:4:DT:O2	3:A:215:THR:HG21	2.03	0.58
1:O:11:DA:H61	2:P:9:DT:H3	1.52	0.58
3:M:73:THR:HG22	3:M:158:GLN:NE2	2.18	0.58
3:I:111:THR:HB	3:I:124:THR:O	2.03	0.58
2:P:11:DT:H2'	2:P:12:DT:C6	2.38	0.57
3:E:153:THR:O	3:E:154:ASP:HB2	2.02	0.57
1:K:8:DA:H1'	3:I:116:PHE:CE1	2.39	0.57
3:E:106:ILE:HG22	3:E:139:TYR:CZ	2.39	0.57
3:E:61:SER:O	3:E:63:ILE:N	2.35	0.57
3:E:133:LYS:HD3	4:F:455:VAL:HG22	1.86	0.57
1:O:13:DG:H1'	1:O:14:DT:H5''	1.87	0.57
3:A:205:LEU:HB2	3:A:213:VAL:HB	1.86	0.57
3:I:118:SER:OG	3:I:119:GLY:N	2.37	0.57
3:I:129:GLU:OE1	3:I:220:ARG:NH2	2.32	0.56
3:A:106:ILE:HD12	4:B:473:HIS:NE2	2.20	0.56
3:A:116:PHE:HE1	3:A:122:VAL:HG23	1.70	0.56
3:A:171:ARG:NH1	3:A:174:GLY:HA3	2.21	0.56
3:A:214:LEU:HD22	3:A:223:ILE:HG23	1.88	0.56
3:E:206:ILE:HD12	3:E:234:LEU:HD21	1.88	0.56
3:A:141:ARG:HH21	3:A:145:LYS:HG3	1.69	0.56
3:M:67:LEU:HD21	3:M:220:ARG:HG3	1.87	0.55
2:L:14:DT:H2''	2:L:15:DT:H5'	1.87	0.55
1:O:6:DA:C2	3:M:71:VAL:HG21	2.41	0.55
2:P:14:DT:H2''	2:P:15:DT:H5'	1.88	0.55
3:A:206:ILE:HD13	3:A:212:ILE:HG23	1.87	0.55
2:P:8:DA:H2''	2:P:9:DT:O5'	2.06	0.55
4:J:503:LEU:O	4:J:506:GLU:HB2	2.07	0.55
3:I:90:ARG:HA	4:J:475:LEU:HD21	1.89	0.55
4:J:461:ASN:ND2	4:J:463:GLU:HG3	2.21	0.55
3:E:64:VAL:HG12	3:I:66:THR:HG22	1.89	0.54
3:E:145:LYS:HD2	4:F:474:LEU:HD11	1.88	0.54
3:M:207:PHE:CE2	3:M:213:VAL:HG23	2.41	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:206:ILE:HD12	3:M:234:LEU:HD21	1.89	0.54
3:I:202:ILE:HD11	3:I:217:ALA:HB2	1.89	0.54
1:K:6:DA:C2	3:I:71:VAL:HG21	2.42	0.54
2:D:14:DT:H2''	2:D:15:DT:H5'	1.89	0.54
1:O:2:DT:H2''	1:O:3:DA:H8	1.72	0.54
3:A:70:ILE:HG12	3:A:126:ALA:O	2.07	0.54
3:E:175:LEU:HD22	3:E:193:LEU:HD21	1.89	0.54
3:A:70:ILE:HG23	3:A:160:ILE:HG12	1.90	0.54
3:A:134:LEU:HA	3:A:137:ARG:HB2	1.89	0.54
2:H:2:DA:H2''	2:H:3:DA:C8	2.43	0.54
3:A:163:SER:HA	3:A:212:ILE:O	2.07	0.54
3:E:85:VAL:HG22	3:E:102:VAL:HG11	1.89	0.54
3:E:74:VAL:HG21	3:E:136:SER:HB3	1.90	0.54
3:A:185:TYR:HB2	3:A:193:LEU:HD12	1.90	0.54
3:A:106:ILE:HG13	3:A:107:ARG:H	1.71	0.53
3:A:195:TYR:HD2	3:A:204:LEU:HD13	1.73	0.53
2:L:16:DA:H4'	3:I:68:GLN:HG3	1.90	0.53
1:C:17:DT:N3	2:D:4:DA:H2	2.06	0.53
3:I:231:TYR:HB3	3:I:232:PRO:HD3	1.90	0.53
2:H:1:DA:H2'	2:H:2:DA:H8	1.72	0.53
4:F:448:THR:HG22	4:F:452:LEU:HD12	1.90	0.53
3:M:71:VAL:HG22	3:M:124:THR:HG22	1.90	0.53
2:L:13:DT:C2'	2:L:14:DT:H5''	2.17	0.53
3:A:137:ARG:HG3	3:A:152:PHE:CE1	2.44	0.52
3:M:178:SER:HB2	3:M:237:PHE:HZ	1.74	0.52
3:M:178:SER:CB	3:M:237:PHE:HZ	2.22	0.52
4:J:470:LEU:O	4:J:473:HIS:HB2	2.10	0.52
3:A:206:ILE:HG23	3:A:212:ILE:HD12	1.92	0.52
1:K:16:DT:H2''	1:K:17:DT:O5'	2.09	0.52
3:M:99:PHE:CE2	3:M:114:LEU:HD22	2.44	0.52
3:M:130:ASP:O	3:M:134:LEU:HB2	2.09	0.52
3:I:109:PRO:O	3:I:111:THR:HG23	2.10	0.52
3:A:166:VAL:HG21	3:A:170:ILE:HD11	1.92	0.52
2:L:15:DT:H2''	2:L:16:DA:C8	2.45	0.52
3:A:106:ILE:HG22	3:A:139:TYR:OH	2.10	0.52
3:A:95:ASN:HD22	3:A:98:ARG:HB2	1.75	0.52
3:I:129:GLU:O	3:I:132:SER:HB3	2.10	0.51
1:C:14:DT:H3	2:D:6:DA:H2	1.58	0.51
3:E:220:ARG:HG2	3:E:224:TYR:CE2	2.45	0.51
2:L:17:DT:H1'	3:I:207:PHE:CZ	2.45	0.51
1:G:8:DA:H1'	3:E:116:PHE:CE1	2.45	0.51
3:I:74:VAL:CG1	3:I:121:MET:CE	2.88	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:73:THR:HG22	3:M:158:GLN:HE21	1.75	0.51
3:M:215:THR:OG1	3:M:216:GLY:N	2.44	0.51
3:M:137:ARG:NH2	4:N:458:ASP:O	2.43	0.51
3:A:155:PHE:HE2	4:B:452:LEU:HD21	1.76	0.51
3:A:88:HIS:O	3:A:89:ALA:HB2	2.11	0.51
3:A:99:PHE:CD2	3:A:101:ALA:HB3	2.45	0.51
3:I:97:LYS:HG3	4:J:494:PHE:HB2	1.92	0.51
3:E:106:ILE:HG13	3:E:108:GLU:H	1.77	0.50
3:I:87:LEU:HD13	4:J:484:GLU:HB2	1.92	0.50
3:I:204:LEU:HD23	3:I:206:ILE:HD11	1.93	0.50
3:A:140:ALA:HB3	4:B:462:LEU:HD22	1.92	0.50
3:A:105:ARG:HD3	3:A:112:THR:HG23	1.92	0.50
3:E:75:THR:HG23	3:E:120:LYS:HD3	1.93	0.50
4:F:440:ARG:NH1	4:F:440:ARG:HG3	2.27	0.50
3:M:221:GLU:O	3:M:224:TYR:N	2.44	0.50
4:B:441:ASN:HB3	4:B:444:LEU:HD12	1.93	0.50
3:A:129:GLU:OE2	4:B:448:THR:HA	2.12	0.50
2:P:16:DA:H2	3:M:213:VAL:CG1	2.24	0.50
3:E:71:VAL:HG13	3:E:124:THR:HG22	1.92	0.50
1:C:17:DT:H2'	1:C:18:DT:C6	2.47	0.50
3:A:111:THR:CG2	3:A:135:ALA:HB2	2.40	0.50
1:K:6:DA:H2	3:I:71:VAL:HG21	1.77	0.50
3:E:133:LYS:HG3	3:E:155:PHE:CE2	2.47	0.49
3:A:137:ARG:HG2	4:B:462:LEU:HD23	1.94	0.49
3:M:133:LYS:HD2	4:N:455:VAL:HG13	1.93	0.49
1:C:5:DA:C6	1:C:6:DA:N6	2.81	0.49
3:I:143:ILE:HG22	3:I:150:ALA:HB2	1.93	0.49
3:A:129:GLU:HG2	4:B:448:THR:HG23	1.94	0.49
3:I:129:GLU:CD	3:I:220:ARG:HH21	2.15	0.49
3:A:180:GLY:HA2	3:A:183:SER:HB2	1.94	0.49
2:H:6:DA:C2	2:H:7:DC:C2	3.00	0.49
3:I:76:LEU:HD21	3:I:140:ALA:HA	1.94	0.49
3:I:223:ILE:HG22	3:I:224:TYR:N	2.27	0.49
3:E:133:LYS:HD2	4:F:452:LEU:HD23	1.95	0.49
2:D:14:DT:C7	2:D:15:DT:H73	2.43	0.49
4:F:458:ASP:OD1	4:F:461:ASN:N	2.41	0.49
3:A:139:TYR:N	3:A:139:TYR:CD1	2.80	0.49
3:E:165:ASP:HB2	3:E:211:LYS:HD2	1.94	0.49
3:E:159:ASN:HA	3:E:217:ALA:O	2.13	0.49
3:A:137:ARG:HH12	4:B:462:LEU:HA	1.78	0.48
4:F:448:THR:HG22	4:F:452:LEU:HD11	1.95	0.48
2:L:16:DA:C4'	3:I:68:GLN:HG3	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:470:LEU:HA	4:B:473:HIS:HD2	1.78	0.48
1:O:5:DA:H2''	1:O:6:DA:H5'	1.95	0.48
3:E:94:TYR:CZ	3:E:96:PRO:HG3	2.48	0.48
3:M:223:ILE:O	3:M:226:ALA:HB3	2.13	0.48
4:F:435:GLY:CA	3:I:128:SER:HB3	2.38	0.48
3:A:121:MET:HG3	3:A:123:VAL:HG23	1.96	0.48
4:J:454:LYS:HD3	4:J:455:VAL:H	1.78	0.48
3:I:219:GLN:N	3:I:222:GLU:OE1	2.46	0.48
3:A:102:VAL:HB	3:A:115:ILE:CG2	2.42	0.48
1:O:10:DA:C2	1:O:11:DA:C6	3.01	0.48
2:H:7:DC:H2''	2:H:8:DA:C8	2.49	0.48
3:E:219:GLN:HG2	3:E:222:GLU:OE2	2.14	0.48
3:M:203:VAL:O	3:M:204:LEU:HD23	2.14	0.48
2:D:14:DT:H5''	3:A:112:THR:OG1	2.13	0.48
3:E:93:GLU:HG3	3:E:103:ILE:HB	1.95	0.48
3:E:184:SER:HB2	3:E:194:ILE:HD12	1.95	0.48
3:E:133:LYS:HG3	3:E:155:PHE:CD2	2.48	0.48
3:E:221:GLU:CG	4:F:447:THR:HG22	2.44	0.48
2:L:6:DA:C2	2:L:7:DC:C2	3.02	0.48
3:M:75:THR:HG23	3:M:120:LYS:HD3	1.95	0.47
3:A:195:TYR:CD2	3:A:204:LEU:HD13	2.49	0.47
3:E:69:ASN:HD21	3:E:125:GLY:H	1.62	0.47
3:E:90:ARG:HD3	3:E:90:ARG:HA	1.62	0.47
3:I:107:ARG:O	3:I:108:GLU:CG	2.61	0.47
3:I:74:VAL:CG1	3:I:121:MET:HE3	2.42	0.47
3:M:110:LYS:O	3:M:111:THR:HG23	2.14	0.47
3:M:161:VAL:HG22	3:M:215:THR:HB	1.97	0.47
3:I:116:PHE:O	3:I:117:ALA:C	2.52	0.47
3:M:206:ILE:HG23	3:M:212:ILE:CD1	2.44	0.47
3:A:186:GLU:HB2	3:A:189:LEU:HB3	1.95	0.47
3:A:88:HIS:HA	4:B:475:LEU:CD1	2.44	0.47
3:A:205:LEU:O	3:A:212:ILE:HA	2.15	0.47
4:F:502:ARG:HA	4:F:505:GLN:HB2	1.97	0.47
3:A:88:HIS:HA	4:B:475:LEU:HD11	1.96	0.47
3:M:197:MET:HB3	3:M:202:ILE:H	1.79	0.46
3:A:217:ALA:HB3	3:A:223:ILE:HG13	1.97	0.46
1:O:6:DA:H2''	1:O:7:DA:O5'	2.15	0.46
3:A:159:ASN:HD21	3:A:216:GLY:H	1.63	0.46
3:I:74:VAL:HG13	3:I:121:MET:HE2	1.98	0.46
1:C:7:DA:C2'	1:C:8:DA:H5'	2.45	0.46
3:I:217:ALA:HB3	3:I:223:ILE:HD12	1.98	0.46
3:I:106:ILE:HG12	3:I:108:GLU:H	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:195:TYR:HB3	3:I:204:LEU:HB2	1.97	0.46
3:I:70:ILE:HG23	3:I:160:ILE:HG12	1.97	0.46
2:H:14:DT:H1'	3:E:69:ASN:OD1	2.16	0.46
4:B:437:TYR:CD2	4:B:438:CYS:N	2.84	0.46
3:E:169:PRO:HA	3:E:208:VAL:O	2.15	0.46
3:E:87:LEU:HD13	4:F:484:GLU:HB2	1.97	0.46
3:M:63:ILE:HD13	3:M:166:VAL:HG12	1.97	0.46
3:E:138:LYS:HG2	4:F:470:LEU:HD12	1.98	0.46
3:I:145:LYS:HB3	4:J:474:LEU:HD21	1.97	0.46
2:H:13:DT:OP1	3:E:98:ARG:NH2	2.42	0.46
3:I:90:ARG:HG2	3:I:91:ASN:ND2	2.31	0.46
3:A:70:ILE:HG13	3:A:128:SER:O	2.16	0.46
1:C:2:DT:O4	1:C:3:DA:N6	2.49	0.46
3:M:140:ALA:HA	3:M:143:ILE:HD12	1.97	0.46
3:I:199:LYS:HA	3:I:200:PRO:HA	1.79	0.46
3:I:235:SER:O	3:I:236:GLU:C	2.52	0.46
3:M:182:PHE:CD2	3:M:196:ARG:O	2.69	0.45
3:I:115:ILE:HD13	3:I:143:ILE:HD11	1.98	0.45
3:I:230:ILE:HG13	3:I:230:ILE:O	2.15	0.45
3:M:185:TYR:HB2	3:M:193:LEU:HD23	1.97	0.45
3:A:206:ILE:HG23	3:A:212:ILE:CD1	2.46	0.45
2:P:16:DA:C2	3:M:213:VAL:CG1	2.98	0.45
3:M:69:ASN:HD21	3:M:125:GLY:N	2.13	0.45
4:F:441:ASN:OD1	4:F:441:ASN:O	2.33	0.45
3:A:104:MET:O	3:A:112:THR:O	2.34	0.45
3:A:141:ARG:O	3:A:145:LYS:HB2	2.17	0.45
4:B:500:SER:HA	4:B:503:LEU:HD12	1.99	0.45
3:E:115:ILE:HG13	3:E:121:MET:HG3	1.99	0.45
1:O:6:DA:N3	3:M:71:VAL:HG11	2.32	0.45
1:O:8:DA:H61	2:P:12:DT:H3	1.65	0.45
1:O:8:DA:N6	2:P:12:DT:H3	2.14	0.45
3:I:90:ARG:HB3	4:J:473:HIS:O	2.17	0.45
1:O:2:DT:H2''	1:O:3:DA:O5'	2.17	0.45
2:P:11:DT:C2'	2:P:12:DT:C6	3.00	0.45
4:J:463:GLU:O	4:J:466:ASP:HB2	2.17	0.44
1:C:17:DT:N3	2:D:4:DA:C2	2.85	0.44
3:I:231:TYR:HB3	3:I:232:PRO:CD	2.47	0.44
1:K:4:DT:H5''	3:I:194:ILE:HG12	1.99	0.44
3:A:166:VAL:HG22	3:A:210:GLY:O	2.17	0.44
3:A:199:LYS:HA	3:A:200:PRO:HA	1.75	0.44
3:I:61:SER:C	3:I:63:ILE:H	2.20	0.44
3:I:134:LEU:O	3:I:138:LYS:HG3	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:141:ARG:HB3	4:B:470:LEU:HD11	1.98	0.44
2:H:6:DA:H2''	2:H:7:DC:O5'	2.18	0.44
1:G:13:DG:C2	2:H:8:DA:C2	3.05	0.44
3:E:214:LEU:HD12	3:E:214:LEU:N	2.33	0.44
3:M:80:LEU:HD12	3:M:119:GLY:HA2	1.99	0.44
1:O:1:DC:H42	2:P:19:DG:H1	1.66	0.44
3:M:197:MET:O	3:M:201:LYS:HA	2.18	0.44
3:I:74:VAL:CG1	3:I:121:MET:HE2	2.48	0.44
3:I:159:ASN:HD21	3:I:216:GLY:CA	2.30	0.44
3:E:133:LYS:HB3	4:F:455:VAL:HG21	2.00	0.44
3:E:141:ARG:NH2	3:E:145:LYS:HE3	2.33	0.44
3:A:152:PHE:HB2	4:B:462:LEU:HD21	2.00	0.44
2:H:11:DT:C5	2:H:12:DT:H73	2.53	0.44
3:M:106:ILE:HB	3:M:139:TYR:CE1	2.53	0.43
3:E:168:PHE:CE1	3:E:238:ARG:HB2	2.53	0.43
3:M:206:ILE:HD12	3:M:234:LEU:CD2	2.48	0.43
3:A:196:ARG:HD3	3:A:203:VAL:HG22	2.00	0.43
3:I:159:ASN:HD21	3:I:216:GLY:H	1.64	0.43
3:I:172:LEU:HD22	3:I:193:LEU:HB2	1.98	0.43
3:E:237:PHE:O	3:E:238:ARG:HB2	2.16	0.43
3:I:70:ILE:HA	3:I:159:ASN:O	2.18	0.43
3:M:143:ILE:HG22	3:M:148:PHE:HB2	2.00	0.43
4:F:441:ASN:C	4:F:441:ASN:OD1	2.56	0.43
3:M:70:ILE:N	3:M:126:ALA:O	2.51	0.43
3:I:165:ASP:OD2	3:I:211:LYS:HE2	2.19	0.43
3:A:139:TYR:HD1	3:A:139:TYR:N	2.17	0.43
3:I:138:LYS:HE2	4:J:465:VAL:HB	2.00	0.43
2:P:17:DT:H4'	3:M:207:PHE:CE2	2.54	0.43
4:F:463:GLU:HA	4:F:466:ASP:OD2	2.18	0.43
4:F:504:LYS:C	4:F:506:GLU:H	2.21	0.43
3:A:86:ALA:C	3:A:88:HIS:H	2.21	0.43
4:F:466:ASP:O	4:F:467:ASP:HB3	2.18	0.43
1:C:7:DA:O4'	3:A:158:GLN:HG3	2.19	0.43
2:P:17:DT:H2''	2:P:18:DA:C8	2.54	0.43
1:G:6:DA:C2	3:E:71:VAL:HG21	2.54	0.43
3:A:94:TYR:CZ	3:A:96:PRO:HG3	2.54	0.43
3:A:113:ALA:HA	3:A:122:VAL:O	2.19	0.42
3:M:63:ILE:HB	3:M:227:PHE:CE2	2.54	0.42
3:M:230:ILE:O	3:M:230:ILE:HG12	2.18	0.42
3:A:219:GLN:O	3:A:222:GLU:HB2	2.19	0.42
3:I:165:ASP:OD1	3:I:167:LYS:HD2	2.18	0.42
1:O:17:DT:H2''	1:O:18:DT:O5'	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:116:PHE:CE1	3:A:122:VAL:HG23	2.53	0.42
4:F:470:LEU:C	4:F:470:LEU:HD23	2.40	0.42
3:I:64:VAL:HA	3:I:65:PRO:HD3	1.89	0.42
2:H:13:DT:H2''	2:H:14:DT:H5'	2.02	0.42
3:E:70:ILE:HG23	3:E:160:ILE:HG12	2.00	0.42
2:L:15:DT:H6	2:L:15:DT:H2'	1.64	0.42
3:A:105:ARG:HA	3:A:112:THR:HA	2.01	0.42
4:B:461:ASN:C	4:B:463:GLU:H	2.22	0.42
1:G:16:DT:H2''	1:G:17:DT:H6	1.84	0.42
4:F:441:ASN:O	4:F:442:LEU:C	2.57	0.42
1:C:11:DA:H2''	1:C:12:DT:C6	2.55	0.42
3:I:89:ALA:HB3	3:I:92:ALA:HB2	2.00	0.42
1:O:5:DA:OP1	3:M:196:ARG:NH1	2.51	0.42
3:I:166:VAL:HG22	3:I:210:GLY:O	2.20	0.42
1:G:3:DA:H2''	1:G:4:DT:H5'	2.01	0.42
3:M:133:LYS:HB3	4:N:455:VAL:HG21	2.02	0.41
3:A:82:LEU:O	3:A:83:LYS:C	2.58	0.41
3:A:186:GLU:HA	3:A:187:PRO:HD3	1.91	0.41
3:M:70:ILE:HG23	3:M:157:ILE:CG2	2.50	0.41
4:F:444:LEU:HA	4:F:444:LEU:HD23	1.85	0.41
1:O:4:DT:H3	2:P:16:DA:N6	2.14	0.41
3:E:220:ARG:CG	3:E:224:TYR:CE2	3.03	0.41
3:M:102:VAL:O	3:M:115:ILE:HD12	2.20	0.41
3:I:111:THR:HG22	3:I:126:ALA:N	2.35	0.41
3:M:161:VAL:HG22	3:M:215:THR:CB	2.51	0.41
4:J:475:LEU:HB3	4:J:479:ALA:HB3	2.03	0.41
3:I:230:ILE:O	3:I:233:VAL:HB	2.20	0.41
3:A:197:MET:O	3:A:201:LYS:HA	2.20	0.41
3:M:199:LYS:HA	3:M:200:PRO:HA	1.84	0.41
3:M:95:ASN:HA	3:M:96:PRO:HD3	1.88	0.41
3:A:76:LEU:HB3	3:A:150:ALA:HB1	2.03	0.41
4:F:500:SER:O	4:F:503:LEU:HB2	2.20	0.41
3:A:99:PHE:HD2	3:A:101:ALA:HB3	1.84	0.41
3:M:113:ALA:HA	3:M:122:VAL:O	2.21	0.41
3:M:159:ASN:ND2	3:M:216:GLY:H	2.19	0.41
3:I:109:PRO:HD2	3:I:135:ALA:HB2	2.03	0.41
4:B:437:TYR:HD2	4:B:438:CYS:H	1.68	0.41
1:G:5:DA:H8	1:G:5:DA:H2'	1.81	0.41
3:E:211:LYS:HG2	3:E:211:LYS:H	1.70	0.41
3:A:155:PHE:CE2	4:B:452:LEU:HD21	2.56	0.41
3:M:123:VAL:HG12	3:M:123:VAL:O	2.21	0.41
3:M:182:PHE:H	3:M:182:PHE:HD1	1.66	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:205:LEU:HB2	3:M:213:VAL:HB	2.03	0.40
2:P:11:DT:C6	2:P:12:DT:H72	2.56	0.40
3:M:233:VAL:HG13	3:M:233:VAL:O	2.20	0.40
2:L:3:DA:C2	2:L:4:DA:C4	3.09	0.40
4:B:470:LEU:HA	4:B:473:HIS:CD2	2.56	0.40
3:I:214:LEU:HD21	3:I:227:PHE:HB2	2.02	0.40
3:I:178:SER:HG	3:I:237:PHE:HZ	1.68	0.40
3:E:230:ILE:O	3:E:233:VAL:HB	2.22	0.40
3:I:137:ARG:HH22	4:J:458:ASP:HB3	1.86	0.40
3:M:178:SER:CB	3:M:237:PHE:CZ	3.03	0.40
1:C:1:DC:H2'	1:C:2:DT:C6	2.57	0.40
3:M:106:ILE:HD13	3:M:108:GLU:H	1.87	0.40
3:I:169:PRO:HG2	3:I:239:LYS:HB3	2.02	0.40
3:E:95:ASN:C	3:E:95:ASN:ND2	2.70	0.40
2:H:17:DT:H1'	3:E:207:PHE:CE2	2.56	0.40
3:I:230:ILE:HG13	3:I:233:VAL:HB	2.03	0.40
3:I:117:ALA:O	3:I:118:SER:C	2.59	0.40
2:D:1:DA:H2''	2:D:2:DA:C5'	2.50	0.40
3:A:161:VAL:HA	3:A:215:THR:HA	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	
3	A	178/180 (99%)	140 (79%)	29 (16%)	9 (5%)	3	16
3	E	178/180 (99%)	154 (86%)	15 (8%)	9 (5%)	3	16
3	I	178/180 (99%)	159 (89%)	12 (7%)	7 (4%)	5	23
3	M	178/180 (99%)	154 (86%)	20 (11%)	4 (2%)	10	43
4	B	70/72 (97%)	58 (83%)	11 (16%)	1 (1%)	16	58
4	F	70/72 (97%)	56 (80%)	12 (17%)	2 (3%)	7	33
4	J	51/72 (71%)	46 (90%)	4 (8%)	1 (2%)	11	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N	51/72 (71%)	47 (92%)	4 (8%)	0	100	100
All	All	954/1008 (95%)	814 (85%)	107 (11%)	33 (4%)	6	27

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	106	ILE
3	E	90	ARG
3	E	118	SER
3	E	150	ALA
3	E	238	ARG
4	F	442	LEU
3	I	89	ALA
3	I	118	SER
3	I	150	ALA
3	M	206	ILE
3	A	149	ALA
3	E	62	GLY
3	E	220	ARG
3	I	110	LYS
3	I	201	LYS
4	J	493	ASP
3	M	93	GLU
3	M	150	ALA
3	A	89	ALA
3	A	98	ARG
3	A	110	LYS
3	A	114	LEU
3	A	146	ILE
3	A	150	ALA
3	E	92	ALA
3	M	149	ALA
4	B	476	ASN
3	E	119	GLY
3	I	119	GLY
3	A	87	LEU
3	E	179	HIS
4	F	505	GLN
3	I	90	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	152/152 (100%)	124 (82%)	28 (18%)	2	11
3	E	152/152 (100%)	135 (89%)	17 (11%)	9	31
3	I	152/152 (100%)	121 (80%)	31 (20%)	2	8
3	M	152/152 (100%)	119 (78%)	33 (22%)	1	6
4	B	67/67 (100%)	50 (75%)	17 (25%)	1	3
4	F	67/67 (100%)	55 (82%)	12 (18%)	2	12
4	J	49/67 (73%)	36 (74%)	13 (26%)	1	3
4	N	49/67 (73%)	41 (84%)	8 (16%)	3	15
All	All	840/876 (96%)	681 (81%)	159 (19%)	2	10

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	61	SER
3	A	63	ILE
3	A	70	ILE
3	A	78	CYS
3	A	80	LEU
3	A	91	ASN
3	A	98	ARG
3	A	107	ARG
3	A	108	GLU
3	A	110	LYS
3	A	120	LYS
3	A	130	ASP
3	A	132	SER
3	A	134	LEU
3	A	136	SER
3	A	139	TYR
3	A	145	LYS
3	A	154	ASP
3	A	175	LEU
3	A	181	THR
3	A	184	SER

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Mol	Chain	Res	Type
3	A	186	GLU
3	A	189	LEU
3	A	193	LEU
3	A	198	VAL
3	A	214	LEU
3	A	215	THR
3	A	218	LYS
4	B	442	LEU
4	B	448	THR
4	B	449	ASP
4	B	461	ASN
4	B	464	ASP
4	B	468	GLU
4	B	470	LEU
4	B	474	LEU
4	B	475	LEU
4	B	478	GLU
4	B	482	LEU
4	B	483	LYS
4	B	485	ARG
4	B	488	ILE
4	B	499	GLU
4	B	501	LYS
4	B	504	LYS
3	E	69	ASN
3	E	79	ARG
3	E	80	LEU
3	E	85	VAL
3	E	90	ARG
3	E	95	ASN
3	E	106	ILE
3	E	132	SER
3	E	134	LEU
3	E	136	SER
3	E	170	ILE
3	E	184	SER
3	E	193	LEU
3	E	194	ILE
3	E	199	LYS
3	E	201	LYS
3	E	211	LYS
4	F	442	LEU

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Mol	Chain	Res	Type
4	F	447	THR
4	F	455	VAL
4	F	475	LEU
4	F	477	GLU
4	F	494	PHE
4	F	497	GLU
4	F	498	GLN
4	F	499	GLU
4	F	500	SER
4	F	501	LYS
4	F	502	ARG
3	I	64	VAL
3	I	73	THR
3	I	79	ARG
3	I	83	LYS
3	I	90	ARG
3	I	98	ARG
3	I	106	ILE
3	I	107	ARG
3	I	110	LYS
3	I	127	LYS
3	I	133	LYS
3	I	134	LEU
3	I	136	SER
3	I	142	ILE
3	I	143	ILE
3	I	144	GLN
3	I	145	LYS
3	I	159	ASN
3	I	167	LYS
3	I	170	ILE
3	I	173	GLU
3	I	177	PHE
3	I	178	SER
3	I	181	THR
3	I	188	GLU
3	I	198	VAL
3	I	214	LEU
3	I	218	LYS
3	I	220	ARG
3	I	223	ILE
3	I	230	ILE

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Mol	Chain	Res	Type
4	J	454	LYS
4	J	455	VAL
4	J	466	ASP
4	J	469	GLU
4	J	477	GLU
4	J	478	GLU
4	J	481	LYS
4	J	485	ARG
4	J	496	LEU
4	J	498	GLN
4	J	499	GLU
4	J	502	ARG
4	J	503	LEU
3	M	68	GLN
3	M	70	ILE
3	M	82	LEU
3	M	90	ARG
3	M	95	ASN
3	M	97	LYS
3	M	106	ILE
3	M	111	THR
3	M	121	MET
3	M	123	VAL
3	M	127	LYS
3	M	131	ASP
3	M	132	SER
3	M	134	LEU
3	M	153	THR
3	M	157	ILE
3	M	158	GLN
3	M	167	LYS
3	M	173	GLU
3	M	175	LEU
3	M	182	PHE
3	M	188	GLU
3	M	189	LEU
3	M	201	LYS
3	M	206	ILE
3	M	208	VAL
3	M	215	THR
3	M	218	LYS
3	M	221	GLU

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Mol	Chain	Res	Type
3	M	233	VAL
3	M	235	SER
3	M	238	ARG
3	M	240	MET
4	N	457	ASP
4	N	468	GLU
4	N	469	GLU
4	N	474	LEU
4	N	486	ILE
4	N	495	LEU
4	N	498	GLN
4	N	501	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	95	ASN
3	A	159	ASN
3	E	69	ASN
3	E	95	ASN
3	E	158	GLN
4	F	498	GLN
4	F	505	GLN
3	I	68	GLN
3	I	88	HIS
3	I	91	ASN
3	I	159	ASN
3	I	225	GLN
4	J	461	ASN
4	J	473	HIS
4	J	498	GLN
3	M	69	ASN
3	M	88	HIS
3	M	158	GLN
3	M	159	ASN
4	N	498	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	19/19 (100%)	0.02	0 100 100	21, 27, 30, 31	0
1	G	19/19 (100%)	-0.17	0 100 100	24, 27, 32, 32	0
1	K	19/19 (100%)	0.07	0 100 100	24, 29, 32, 32	0
1	O	19/19 (100%)	-0.07	0 100 100	26, 29, 31, 32	0
2	D	19/19 (100%)	0.03	0 100 100	25, 28, 30, 30	0
2	H	19/19 (100%)	-0.01	0 100 100	24, 29, 36, 37	0
2	L	19/19 (100%)	0.19	0 100 100	24, 27, 32, 32	0
2	P	19/19 (100%)	-0.14	0 100 100	25, 27, 30, 32	0
3	A	180/180 (100%)	0.19	0 100 100	24, 28, 30, 31	0
3	E	180/180 (100%)	0.26	0 100 100	23, 28, 33, 39	0
3	I	180/180 (100%)	0.24	0 100 100	22, 28, 33, 39	0
3	M	180/180 (100%)	0.12	1 (0%) 86 47	22, 28, 30, 31	0
4	B	72/72 (100%)	0.25	2 (2%) 50 22	27, 29, 30, 31	0
4	F	72/72 (100%)	0.12	0 100 100	23, 29, 33, 34	0
4	J	53/72 (73%)	0.01	2 (3%) 38 18	24, 29, 33, 34	0
4	N	53/72 (73%)	0.68	6 (11%) 6 3	28, 29, 29, 30	0
All	All	1122/1160 (96%)	0.19	11 (0%) 79 38	21, 28, 32, 39	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	496	LEU	3.2
4	N	503	LEU	2.7
3	M	87	LEU	2.6
4	B	505	GLN	2.5
4	N	472	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	N	477	GLU	2.3
4	J	503	LEU	2.2
4	N	500	SER	2.2
4	J	506	GLU	2.1
4	N	488	ILE	2.0
4	B	442	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.