



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:27 PM GMT

PDB ID : 4RVE  
Title : THE CRYSTAL STRUCTURE OF ECORV ENDONUCLEASE AND OF ITS COMPLEXES WITH COGNATE AND NON-COGNATE DNA SEGMENTS  
Authors : Winkler, F.K.; Banner, D.W.; Oefner, C.; Tsernoglou, D.; Brown, R.S.; Heathman, S.P.; Bryan, R.K.; Martin, P.D.; Petratos, K.; Wilso, K.S.  
Deposited on : 1993-02-18  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

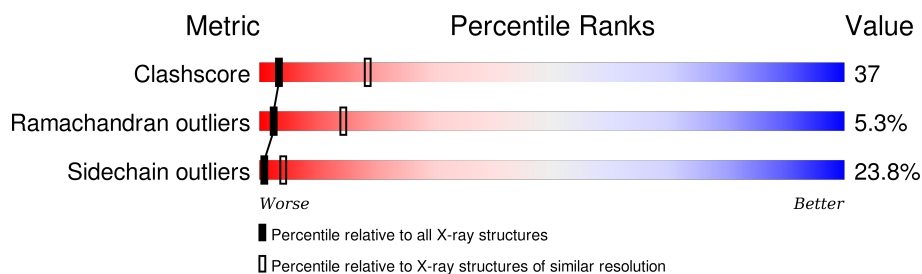
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	10	
1	E	10	
1	F	10	
2	A	244	
2	B	244	
2	C	244	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6590 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 DNA chain called DNA (5'-D(\*GP\*GP\*GP\*AP\*TP\*AP\*TP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			
1	E	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			
1	F	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			

- Molecule 2 is a protein called PROTEIN (ECO RV (E.C.3.1.21.4)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	240	Total	C	N	O	S	202	0	0
			1987	1280	330	376	1			
2	B	240	Total	C	N	O	S	205	0	0
			1987	1280	330	376	1			
2	C	240	Total	C	N	O	S	204	0	0
			1987	1280	330	376	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	4	Total	O	0	0
			4	4		
3	C	8	Total	O	0	0
			8	8		
3	D	1	Total	O	0	0
			1	1		
3	E	2	Total	O	0	0
			2	2		
3	F	1	Total	O	0	0
			1	1		

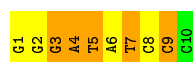
### 3 Residue-property plots [i](#)

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.

Note EDS was not executed.

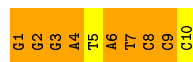
- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*AP\*TP\*AP\*TP\*CP\*CP\*C)-3')

Chain D: 



- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*AP\*TP\*AP\*TP\*CP\*CP\*C)-3')

Chain E: 



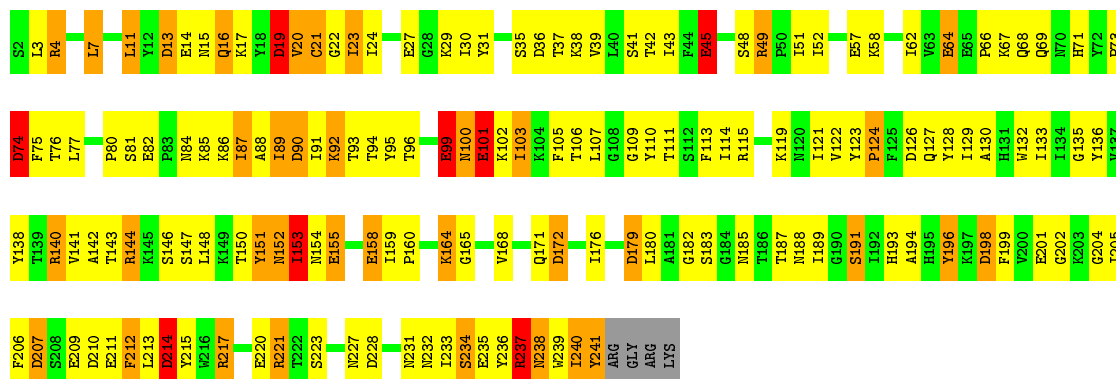
- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*AP\*TP\*AP\*TP\*CP\*CP\*C)-3')

Chain F: 

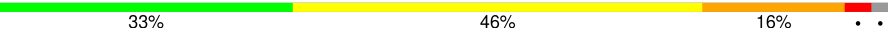


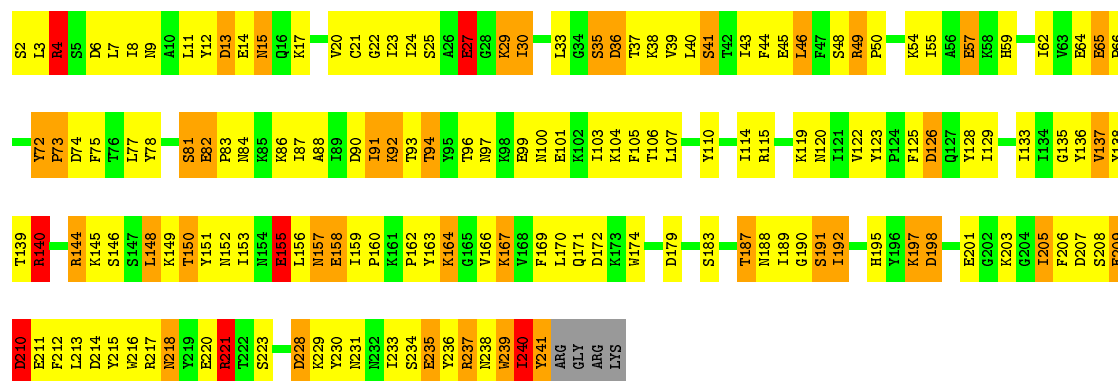
- Molecule 2: PROTEIN (ECO RV (E.C.3.1.21.4))

Chain A: 



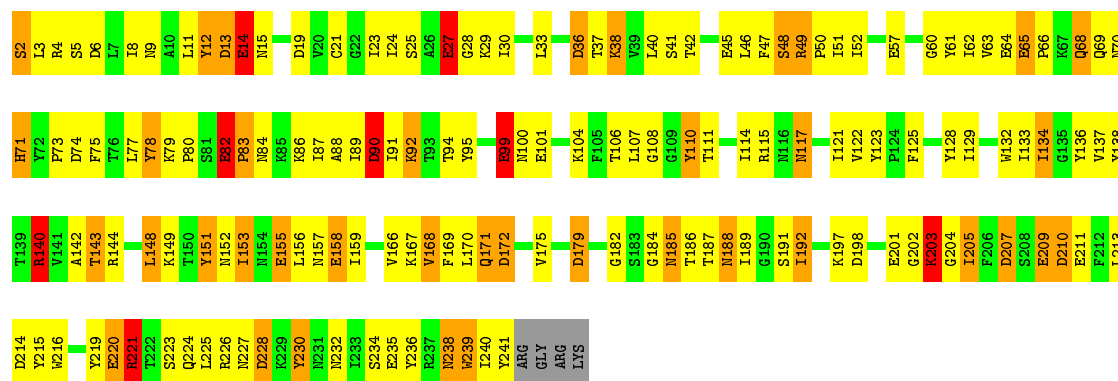
- Molecule 2: PROTEIN (ECO RV (E.C.3.1.21.4))

Chain B:  33% 46% 16% . .



• Molecule 2: PROTEIN (ECO RV (E.C.3.1.21.4))

Chain C:  34% 45% 16% . .



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.20 Å 78.40 Å 371.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 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	D	1.71	2/226 (0.9%)	2.22	21/347 (6.1%)
1	E	1.94	6/226 (2.7%)	2.20	16/347 (4.6%)
1	F	1.83	6/226 (2.7%)	2.14	18/347 (5.2%)
2	A	1.06	13/2038 (0.6%)	1.38	32/2760 (1.2%)
2	B	1.09	16/2038 (0.8%)	1.40	30/2760 (1.1%)
2	C	1.10	13/2038 (0.6%)	1.35	26/2760 (0.9%)
All	All	1.18	56/6792 (0.8%)	1.49	143/9321 (1.5%)

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
2	B	1	0

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	DC	C3'-O3'	-10.12	1.30	1.44
2	C	45	GLU	CD-OE2	8.93	1.35	1.25
1	F	9	DC	C3'-O3'	-7.66	1.33	1.44
2	C	65	GLU	CD-OE1	7.46	1.33	1.25
2	A	220	GLU	CD-OE2	7.36	1.33	1.25
2	A	155	GLU	CD-OE1	7.30	1.33	1.25
2	C	64	GLU	CD-OE1	7.09	1.33	1.25
2	C	158	GLU	CD-OE2	6.96	1.33	1.25
2	C	220	GLU	CD-OE2	6.80	1.33	1.25
1	E	8	DC	C3'-O3'	-6.68	1.35	1.44
2	A	101	GLU	CD-OE2	6.50	1.32	1.25
2	B	158	GLU	CD-OE2	6.50	1.32	1.25
2	B	211	GLU	CD-OE2	6.48	1.32	1.25
2	C	209	GLU	CD-OE2	6.46	1.32	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	235	GLU	CD-OE2	6.45	1.32	1.25
2	B	201	GLU	CD-OE2	6.38	1.32	1.25
2	C	101	GLU	CD-OE1	6.35	1.32	1.25
1	F	2	DG	C3'-O3'	-6.33	1.35	1.44
2	B	45	GLU	CD-OE2	6.29	1.32	1.25
2	A	235	GLU	CD-OE1	6.25	1.32	1.25
2	A	64	GLU	CD-OE2	6.15	1.32	1.25
2	B	155	GLU	CD-OE1	6.08	1.32	1.25
2	C	82	GLU	CD-OE2	6.07	1.32	1.25
2	B	65	GLU	CD-OE1	6.07	1.32	1.25
2	B	209	GLU	CD-OE1	6.00	1.32	1.25
2	A	201	GLU	CD-OE2	6.00	1.32	1.25
2	A	82	GLU	CD-OE2	5.94	1.32	1.25
1	D	9	DC	C1'-N1	-5.87	1.39	1.47
2	C	155	GLU	CD-OE1	5.83	1.32	1.25
2	B	64	GLU	CD-OE1	5.81	1.32	1.25
1	F	3	DG	C3'-O3'	-5.76	1.36	1.44
1	E	7	DT	C3'-O3'	-5.75	1.36	1.44
2	A	45	GLU	CD-OE1	5.73	1.31	1.25
2	B	57	GLU	CD-OE1	5.60	1.31	1.25
2	B	82	GLU	CD-OE1	5.57	1.31	1.25
2	B	99	GLU	CD-OE2	5.47	1.31	1.25
2	A	209	GLU	CD-OE1	5.46	1.31	1.25
2	A	27	GLU	CD-OE2	5.44	1.31	1.25
1	F	4	DA	O3'-P	5.43	1.67	1.61
1	F	5	DT	C3'-O3'	-5.43	1.36	1.44
2	B	14	GLU	CD-OE2	5.36	1.31	1.25
2	C	57	GLU	CD-OE2	5.36	1.31	1.25
1	E	2	DG	P-O5'	5.35	1.65	1.59
2	B	101	GLU	CD-OE2	5.35	1.31	1.25
2	A	57	GLU	CD-OE1	5.34	1.31	1.25
2	B	27	GLU	CD-OE1	5.32	1.31	1.25
1	E	3	DG	N1-C2	-5.32	1.33	1.37
2	A	14	GLU	CD-OE1	5.26	1.31	1.25
1	E	9	DC	N3-C4	-5.26	1.30	1.33
2	C	27	GLU	CD-OE1	5.23	1.31	1.25
2	A	99	GLU	CD-OE2	5.23	1.31	1.25
1	F	4	DA	C3'-O3'	5.21	1.50	1.44
2	C	99	GLU	CD-OE1	5.19	1.31	1.25
1	E	6	DA	N9-C4	5.19	1.41	1.37
2	B	220	GLU	CD-OE2	5.13	1.31	1.25
2	C	14	GLU	CD-OE2	5.09	1.31	1.25



All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	DC	C2-N1-C1'	11.94	131.93	118.80
1	E	10	DC	C6-N1-C1'	-10.68	107.99	120.80
1	F	4	DA	C8-N9-C1'	-10.49	108.82	127.70
1	F	4	DA	C4-N9-C1'	9.98	144.27	126.30
1	D	2	DG	P-O3'-C3'	9.93	131.61	119.70
1	D	5	DT	O4'-C4'-C3'	-9.72	100.17	106.00
1	D	2	DG	C8-N9-C1'	9.40	139.22	127.00
1	D	9	DC	C2-N1-C1'	-8.97	108.93	118.80
2	B	74	ASP	CB-CG-OD1	-8.69	110.48	118.30
1	F	7	DT	O4'-C1'-N1	8.56	113.99	108.00
1	D	2	DG	C4-N9-C1'	-8.45	115.52	126.50
2	B	207	ASP	CB-CG-OD2	-8.14	110.97	118.30
2	A	217	ARG	NE-CZ-NH2	-8.07	116.26	120.30
2	B	210	ASP	CB-CG-OD1	-8.06	111.05	118.30
1	D	3	DG	C8-N9-C1'	7.96	137.35	127.00
1	E	6	DA	O4'-C4'-C3'	-7.88	101.27	106.00
2	A	90	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	E	2	DG	C4-N9-C1'	7.83	136.67	126.50
1	F	5	DT	C2-N1-C1'	-7.82	105.69	118.20
1	F	5	DT	C6-N1-C1'	7.81	132.12	120.40
1	D	9	DC	O4'-C1'-N1	-7.79	102.55	108.00
1	E	1	DG	O4'-C1'-N9	-7.62	102.67	108.00
1	E	10	DC	O4'-C1'-N1	7.55	113.28	108.00
2	A	74	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	E	9	DC	P-O3'-C3'	7.42	128.60	119.70
2	B	221	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	D	3	DG	C4-N9-C1'	-7.29	117.02	126.50
2	C	74	ASP	CB-CG-OD1	7.22	124.80	118.30
1	F	2	DG	C8-N9-C1'	7.22	136.38	127.00
1	F	6	DA	P-O3'-C3'	7.20	128.34	119.70
2	A	217	ARG	NE-CZ-NH1	7.13	123.86	120.30
2	A	74	ASP	CB-CG-OD1	7.13	124.71	118.30
2	A	221	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	F	8	DC	O4'-C1'-N1	-7.08	103.05	108.00
2	A	172	ASP	CB-CG-OD1	7.07	124.67	118.30
2	B	207	ASP	CB-CG-OD1	7.07	124.66	118.30
2	C	214	ASP	CB-CG-OD2	-7.06	111.95	118.30
2	B	90	ASP	CB-CG-OD2	-6.96	112.04	118.30
2	B	74	ASP	CB-CG-OD2	6.95	124.55	118.30
2	B	140	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	B	36	ASP	CB-CG-OD1	6.88	124.49	118.30
2	B	126	ASP	CB-CG-OD2	-6.63	112.33	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	74	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	D	9	DC	C6-N1-C1'	6.59	128.70	120.80
1	D	1	DG	C8-N9-C1'	6.47	135.41	127.00
2	A	36	ASP	CB-CG-OD2	-6.41	112.53	118.30
2	A	210	ASP	CB-CG-OD2	-6.41	112.53	118.30
2	C	36	ASP	CB-CG-OD2	-6.35	112.58	118.30
2	C	207	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	E	8	DC	P-O3'-C3'	-6.33	112.10	119.70
2	B	214	ASP	CB-CG-OD1	6.32	123.98	118.30
1	E	2	DG	C8-N9-C4	-6.25	103.90	106.40
2	A	198	ASP	CB-CG-OD2	-6.23	112.69	118.30
2	B	90	ASP	CB-CG-OD1	6.22	123.90	118.30
1	F	7	DT	C3'-C2'-C1'	-6.22	95.04	102.50
2	C	90	ASP	CB-CG-OD2	-6.21	112.71	118.30
2	B	198	ASP	CB-CG-OD2	6.20	123.88	118.30
2	B	228	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	B	198	ASP	CB-CG-OD1	-6.16	112.75	118.30
2	A	36	ASP	CB-CG-OD1	6.16	123.85	118.30
2	B	210	ASP	CB-CG-OD2	6.16	123.84	118.30
2	C	228	ASP	CB-CG-OD1	-6.14	112.78	118.30
1	F	5	DT	P-O5'-C5'	-6.12	111.11	120.90
2	A	4	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	B	96	THR	N-CA-CB	6.11	121.90	110.30
1	D	3	DG	P-O5'-C5'	-6.07	111.19	120.90
1	F	10	DC	P-O5'-C5'	-6.06	111.20	120.90
2	A	126	ASP	CB-CG-OD2	-6.05	112.86	118.30
2	A	228	ASP	CB-CG-OD1	-6.03	112.87	118.30
2	C	13	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	F	4	DA	C5'-C4'-C3'	5.95	124.80	114.10
2	B	214	ASP	CB-CG-OD2	-5.94	112.95	118.30
2	B	13	ASP	CB-CG-OD1	-5.91	112.98	118.30
2	A	126	ASP	CB-CG-OD1	5.86	123.57	118.30
2	A	49	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	A	172	ASP	CB-CG-OD2	-5.84	113.05	118.30
2	A	13	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	E	2	DG	C8-N9-C1'	-5.82	119.43	127.00
1	E	7	DT	O4'-C4'-C3'	5.81	109.49	106.00
2	B	36	ASP	CB-CG-OD2	-5.81	113.07	118.30
2	B	228	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	8	DC	O4'-C1'-N1	5.80	112.06	108.00
1	F	7	DT	O4'-C1'-C2'	-5.80	101.26	105.90
1	D	7	DT	P-O3'-C3'	5.78	126.64	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	221	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	6	DA	O4'-C1'-N9	5.73	112.01	108.00
2	C	214	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	3	DG	P-O3'-C3'	5.70	126.54	119.70
2	A	207	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	A	19	ASP	CB-CG-OD1	5.70	123.43	118.30
2	B	6	ASP	CB-CG-OD1	5.70	123.43	118.30
2	A	124	PRO	N-CA-CB	5.68	110.12	103.30
2	C	78	TYR	CB-CG-CD2	-5.65	117.61	121.00
2	C	221	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	C	207	ASP	CB-CG-OD1	5.63	123.37	118.30
1	E	8	DC	C2-N1-C1'	5.61	124.97	118.80
2	B	6	ASP	CB-CG-OD2	-5.61	113.25	118.30
2	B	13	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	1	DG	C4-N9-C1'	-5.58	119.25	126.50
2	C	140	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	A	228	ASP	CB-CG-OD2	5.56	123.31	118.30
1	F	7	DT	C1'-O4'-C4'	-5.56	104.54	110.10
2	C	172	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	F	2	DG	C8-N9-C4	-5.55	104.18	106.40
2	C	36	ASP	CB-CG-OD1	5.55	123.30	118.30
2	C	228	ASP	CB-CG-OD2	5.55	123.29	118.30
2	A	214	ASP	CB-CG-OD1	5.52	123.27	118.30
2	A	13	ASP	CB-CG-OD1	5.48	123.23	118.30
1	F	2	DG	C4-N9-C1'	-5.44	119.43	126.50
2	C	90	ASP	CB-CG-OD1	5.43	123.19	118.30
2	B	187	THR	N-CA-CB	-5.41	100.01	110.30
2	A	214	ASP	CB-CG-OD2	-5.41	113.43	118.30
2	C	13	ASP	CB-CG-OD1	5.39	123.16	118.30
2	C	210	ASP	CB-CG-OD2	-5.38	113.46	118.30
2	C	6	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	D	4	DA	C1'-O4'-C4'	-5.34	104.76	110.10
1	E	8	DC	C6-N1-C1'	-5.34	114.39	120.80
2	A	21	CYS	CA-CB-SG	-5.28	104.49	114.00
2	B	115	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	A	19	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	E	7	DT	P-O5'-C5'	-5.25	112.49	120.90
2	C	110	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	C	140	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	C	19	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	E	7	DT	P-O3'-C3'	5.22	125.97	119.70
1	D	4	DA	P-O3'-C3'	5.22	125.96	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	230	TYR	N-CA-CB	5.21	119.98	110.60
2	A	179	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	C	179	ASP	CB-CG-OD2	-5.15	113.66	118.30
2	A	90	ASP	CB-CG-OD1	5.15	122.94	118.30
2	A	210	ASP	CB-CG-OD1	5.15	122.93	118.30
2	B	239	TRP	CA-CB-CG	5.14	123.46	113.70
2	A	4	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	C	198	ASP	CB-CG-OD2	-5.11	113.70	118.30
2	B	240	ILE	N-CA-CB	5.09	122.51	110.80
1	D	9	DC	C6-N1-C2	5.08	122.33	120.30
1	F	3	DG	C8-N9-C1'	5.08	133.61	127.00
1	F	2	DG	O4'-C1'-N9	5.08	111.56	108.00
1	D	4	DA	C4'-C3'-C2'	-5.08	98.53	103.10
1	D	8	DC	P-O5'-C5'	-5.06	112.80	120.90
2	B	4	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	E	4	DA	C4'-C3'-C2'	-5.05	98.56	103.10
2	B	126	ASP	CB-CG-OD1	5.02	122.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	240	ILE	CA

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	202	0	114	9	0
1	E	202	0	114	15	0
1	F	202	0	114	3	0
2	A	1987	0	1945	158	0
2	B	1987	0	1945	148	0
2	C	1987	0	1945	119	0
3	A	7	0	0	2	0
3	B	4	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	0	2	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
All	All	6590	0	6177	423	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 37.

All (423) 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:D:7:DT:H4'	2:B:37:THR:HG21	1.35	1.05
2:C:192:ILE:HD11	2:C:205:ILE:HG13	1.39	1.03
1:E:7:DT:H4'	2:A:37:THR:HG21	1.35	1.03
2:A:11:LEU:HD23	2:A:51:ILE:HG21	1.38	1.00
2:C:171:GLN:HE21	2:C:172:ASP:N	1.58	0.99
2:C:11:LEU:HD11	2:C:134:ILE:HD13	1.45	0.94
2:C:171:GLN:NE2	2:C:172:ASP:H	1.68	0.91
2:B:238:ASN:HA	2:B:241:TYR:HE1	1.32	0.91
1:D:7:DT:H4'	2:B:37:THR:CG2	2.01	0.91
2:A:62:ILE:HD12	2:A:80:PRO:HG3	1.52	0.89
2:C:185:ASN:HD22	2:C:186:THR:N	1.72	0.88
2:C:171:GLN:HE21	2:C:172:ASP:H	0.88	0.87
2:A:11:LEU:CD2	2:A:51:ILE:HG21	2.05	0.86
2:A:106:THR:HG22	2:A:182:GLY:HA3	1.57	0.85
1:E:7:DT:H4'	2:A:37:THR:CG2	2.08	0.83
2:B:213:LEU:HD22	2:B:217:ARG:NH2	1.94	0.83
2:B:170:LEU:HD12	2:B:171:GLN:N	1.94	0.82
2:B:151:TYR:CG	2:B:159:ILE:HD11	2.14	0.82
2:B:170:LEU:HD12	2:B:171:GLN:H	1.43	0.81
2:C:2:SER:N	2:C:5:SER:HG	1.79	0.81
2:B:122:VAL:HG12	2:B:123:TYR:CD1	2.15	0.81
2:C:25:SER:OG	2:C:27:GLU:HG2	1.82	0.80
2:C:185:ASN:HD22	2:C:186:THR:H	1.30	0.80
2:A:31:TYR:CD1	2:B:46:LEU:HD11	2.17	0.79
2:B:81:SER:O	2:B:83:PRO:HD3	1.82	0.78
2:A:86:LYS:HB2	2:A:127:GLN:O	1.83	0.78
2:A:123:TYR:HB3	2:A:127:GLN:HE21	1.49	0.77
2:A:39:VAL:HG12	2:A:43:ILE:CD1	2.16	0.76
2:C:151:TYR:HB3	2:C:155:GLU:HB2	1.67	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:152:ASN:OD1	2:C:155:GLU:HG3	1.84	0.76
1:E:6:DA:C2'	1:E:7:DT:H5'	2.16	0.76
2:C:232:ASN:OD1	2:C:235:GLU:HG3	1.85	0.76
2:A:179:ASP:C	2:A:180:LEU:HD23	2.06	0.76
2:A:206:PHE:CE1	2:A:233:ILE:HD12	2.21	0.75
2:A:85:LYS:HG3	2:A:129:ILE:HD11	1.67	0.75
2:B:240:ILE:N	2:B:240:ILE:HD12	2.01	0.74
1:E:8:DC:H2''	1:E:9:DC:C6	2.21	0.74
2:A:206:PHE:CD2	2:A:212:PHE:HB2	2.23	0.73
2:A:49:ARG:HB2	2:A:75:PHE:HZ	1.53	0.73
2:C:23:ILE:CD1	2:C:33:LEU:HD21	2.19	0.73
2:C:236:TYR:O	2:C:239:TRP:HB3	1.89	0.73
2:A:196:TYR:O	2:A:199:PHE:HB2	1.89	0.72
2:A:233:ILE:HG22	3:A:773:HOH:O	1.88	0.72
2:C:8:ILE:HG23	2:C:12:TYR:CE1	2.24	0.72
2:A:42:THR:HG21	2:B:39:VAL:HG21	1.71	0.72
2:C:23:ILE:HD11	2:C:33:LEU:HD21	1.72	0.72
2:B:197:LYS:HE3	2:B:198:ASP:OD1	1.90	0.71
2:B:151:TYR:CB	2:B:159:ILE:HD11	2.19	0.71
2:A:85:LYS:CB	2:A:129:ILE:HD11	2.21	0.70
2:C:37:THR:HA	2:C:40:LEU:HB2	1.71	0.70
2:C:4:ARG:HB2	2:C:132:TRP:CH2	2.26	0.70
2:C:62:ILE:HD11	2:C:80:PRO:HG3	1.73	0.70
2:B:233:ILE:O	2:B:237:ARG:HG3	1.92	0.69
2:B:135:GLY:HA3	2:B:169:PHE:CE2	2.26	0.69
1:E:4:DA:H5'	2:A:119:LYS:NZ	2.07	0.69
2:A:132:TRP:C	2:A:133:ILE:HD13	2.13	0.68
2:B:238:ASN:HA	2:B:241:TYR:CE1	2.22	0.68
2:A:85:LYS:CG	2:A:129:ILE:HD11	2.23	0.67
2:B:8:ILE:CG2	2:B:12:TYR:HE2	2.07	0.67
2:C:49:ARG:HG3	2:C:49:ARG:NH1	2.08	0.67
2:B:236:TYR:O	2:B:239:TRP:HB3	1.94	0.67
1:E:7:DT:C4'	2:A:37:THR:HG21	2.18	0.67
2:A:207:ASP:HB2	2:A:211:GLU:OE1	1.94	0.67
2:B:40:LEU:HD23	2:B:43:ILE:HD13	1.77	0.66
2:A:89:ILE:HD13	2:A:132:TRP:HE3	1.58	0.66
2:C:27:GLU:H	2:C:27:GLU:CD	1.99	0.66
2:C:49:ARG:N	2:C:50:PRO:HD2	2.10	0.66
2:B:149:LYS:HD3	2:B:151:TYR:CZ	2.30	0.66
2:A:39:VAL:HG12	2:A:43:ILE:HD11	1.76	0.66
2:B:231:ASN:ND2	2:B:235:GLU:OE1	2.29	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:171:GLN:HG3	2:A:172:ASP:N	2.11	0.66
2:C:202:GLY:O	2:C:204:GLY:N	2.30	0.65
2:A:238:ASN:N	2:A:238:ASN:OD1	2.29	0.65
2:B:39:VAL:O	2:B:43:ILE:HD12	1.96	0.65
2:B:105:PHE:H	2:B:191:SER:HB3	1.62	0.65
2:A:87:ILE:HG12	2:A:130:ALA:HB3	1.77	0.65
2:B:179:ASP:OD1	2:B:179:ASP:N	2.30	0.65
2:C:49:ARG:HG3	2:C:49:ARG:HH11	1.61	0.65
2:A:85:LYS:HG3	2:A:129:ILE:CD1	2.28	0.64
2:B:100:ASN:ND2	2:B:195:HIS:HD2	1.96	0.64
2:C:66:PRO:HD3	3:C:754:HOH:O	1.97	0.64
2:A:73:PRO:HG2	2:A:75:PHE:O	1.97	0.64
2:C:49:ARG:NH2	2:C:65:GLU:OE1	2.30	0.64
2:A:3:LEU:O	2:A:3:LEU:HD12	1.96	0.64
1:D:4:DA:H4'	2:B:120:ASN:ND2	2.12	0.64
2:A:24:ILE:HG22	2:B:22:GLY:O	1.97	0.64
2:A:123:TYR:HB3	2:A:127:GLN:NE2	2.12	0.63
2:B:3:LEU:O	2:B:7:LEU:HB2	1.97	0.63
2:C:207:ASP:N	2:C:211:GLU:OE1	2.27	0.63
2:B:8:ILE:HG22	2:B:12:TYR:HE2	1.62	0.63
2:A:179:ASP:O	2:A:180:LEU:HD23	1.98	0.63
2:C:49:ARG:NE	2:C:65:GLU:OE2	2.27	0.63
2:C:62:ILE:O	2:C:77:LEU:HA	1.99	0.63
2:B:107:LEU:HD22	2:B:133:ILE:CD1	2.29	0.63
2:A:49:ARG:HB2	2:A:75:PHE:CZ	2.33	0.62
2:A:105:PHE:HB2	2:A:191:SER:HB3	1.80	0.62
2:B:210:ASP:OD1	2:B:210:ASP:N	2.29	0.62
2:A:58:LYS:HG3	2:A:58:LYS:O	2.00	0.62
2:B:159:ILE:HG23	2:B:160:PRO:HD2	1.82	0.62
2:B:100:ASN:HD21	2:B:195:HIS:HD2	1.48	0.62
2:C:108:GLY:O	2:C:188:ASN:HA	2.00	0.61
2:A:194:ALA:HB1	2:A:198:ASP:OD2	2.00	0.61
2:A:106:THR:HG22	2:A:182:GLY:CA	2.29	0.61
2:A:31:TYR:CE1	2:A:150:THR:HG21	2.35	0.61
2:A:164:LYS:HE2	2:A:165:GLY:H	1.65	0.61
1:D:4:DA:N6	2:A:185:ASN:OD1	2.29	0.61
2:B:155:GLU:O	2:B:158:GLU:N	2.29	0.61
2:A:102:LYS:HD2	2:A:193:HIS:HD2	1.66	0.60
2:B:77:LEU:O	2:B:78:TYR:HB3	2.01	0.60
2:A:42:THR:O	2:A:45:GLU:HB2	2.01	0.60
2:C:137:VAL:O	2:C:166:VAL:HA	1.99	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:TYR:HB2	2:B:159:ILE:HD11	1.82	0.60
2:A:68:GLN:N	2:A:68:GLN:OE1	2.33	0.60
2:C:82:GLU:N	2:C:83:PRO:HD3	2.17	0.60
2:A:135:GLY:O	2:A:168:VAL:HA	2.02	0.60
2:C:153:ILE:O	2:C:153:ILE:HG13	2.01	0.59
2:B:46:LEU:HG	2:B:46:LEU:O	2.01	0.59
2:B:29:LYS:NZ	2:B:150:THR:HG22	2.17	0.59
2:A:91:ILE:O	2:A:92:LYS:HD3	2.02	0.59
2:B:179:ASP:HB2	2:B:215:TYR:OH	2.01	0.59
2:A:109:GLY:HA2	2:A:187:THR:O	2.02	0.59
2:C:107:LEU:N	2:C:189:ILE:O	2.29	0.59
1:D:3:DG:O6	2:A:183:SER:HB2	2.03	0.59
2:A:20:VAL:HA	2:B:25:SER:HA	1.85	0.59
2:A:171:GLN:HG2	2:A:176:ILE:CG2	2.33	0.58
2:A:31:TYR:CD1	2:A:150:THR:HG22	2.38	0.58
2:A:113:PHE:CB	2:A:121:ILE:HD12	2.33	0.58
2:A:153:ILE:HG13	2:B:153:ILE:HD13	1.85	0.58
2:C:47:PHE:O	2:C:50:PRO:HG2	2.02	0.58
2:B:40:LEU:HD23	2:B:43:ILE:CD1	2.32	0.58
2:A:91:ILE:HD12	2:A:91:ILE:N	2.18	0.58
2:B:191:SER:OG	2:B:192:ILE:N	2.36	0.58
2:B:3:LEU:HD23	2:B:87:ILE:HD13	1.86	0.58
2:A:122:VAL:HG12	2:A:123:TYR:CD2	2.38	0.58
2:A:187:THR:HG22	2:A:187:THR:O	2.04	0.58
2:A:152:ASN:O	2:A:155:GLU:N	2.35	0.57
2:B:7:LEU:HD12	2:B:55:ILE:HG13	1.86	0.57
2:B:91:ILE:C	2:B:92:LYS:HG2	2.25	0.57
2:A:179:ASP:OD1	2:A:179:ASP:N	2.36	0.57
2:B:187:THR:HG22	2:B:187:THR:O	2.03	0.57
2:A:48:SER:O	2:A:52:ILE:HG13	2.04	0.57
2:A:113:PHE:CG	2:A:121:ILE:HD12	2.39	0.57
2:A:85:LYS:CA	2:A:129:ILE:HD11	2.35	0.57
2:A:164:LYS:HE2	2:A:165:GLY:N	2.20	0.57
2:B:36:ASP:OD1	2:B:38:LYS:HB2	2.05	0.57
2:B:88:ALA:HB2	2:B:128:TYR:CD2	2.40	0.57
2:C:151:TYR:CD1	2:C:151:TYR:N	2.72	0.57
2:A:214:ASP:HB3	2:A:236:TYR:OH	2.05	0.57
2:B:195:HIS:HB3	2:B:197:LYS:HE2	1.86	0.57
2:A:4:ARG:HH12	2:A:172:ASP:CG	2.06	0.57
2:B:54:LYS:O	2:B:57:GLU:HB3	2.04	0.57
2:B:221:ARG:CG	2:B:221:ARG:HH11	2.18	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:LYS:HZ2	2:B:150:THR:HG22	1.70	0.56
2:B:195:HIS:CB	2:B:197:LYS:HE2	2.36	0.56
2:B:174:TRP:CH2	2:B:208:SER:HA	2.39	0.56
2:C:12:TYR:OH	2:C:169:PHE:HA	2.05	0.56
2:C:75:PHE:HE2	2:C:91:ILE:CD1	2.19	0.56
2:C:4:ARG:HB2	2:C:132:TRP:CZ2	2.40	0.56
2:B:189:ILE:HG22	2:B:190:GLY:N	2.19	0.56
2:C:80:PRO:O	2:C:83:PRO:HD3	2.06	0.56
2:B:37:THR:O	2:B:41:SER:OG	2.23	0.56
2:A:213:LEU:HD13	2:A:217:ARG:NH2	2.20	0.55
2:A:211:GLU:OE2	2:A:237:ARG:NH2	2.34	0.55
2:A:180:LEU:N	2:A:180:LEU:HD23	2.21	0.55
2:B:174:TRP:CZ3	2:B:208:SER:HA	2.41	0.55
2:A:102:LYS:HB3	2:A:193:HIS:CD2	2.41	0.55
2:C:171:GLN:HA	2:C:171:GLN:NE2	2.19	0.55
2:C:4:ARG:O	2:C:8:ILE:HG13	2.07	0.55
2:C:11:LEU:HD11	2:C:134:ILE:CD1	2.29	0.55
2:B:33:LEU:HB2	2:B:162:PRO:HG3	1.88	0.55
2:A:86:LYS:O	2:A:128:TYR:HA	2.07	0.55
2:A:102:LYS:HD3	2:A:194:ALA:HA	1.88	0.55
2:B:221:ARG:HG2	2:B:221:ARG:HH11	1.72	0.55
2:B:49:ARG:HB2	2:B:75:PHE:HE2	1.72	0.54
2:B:229:LYS:HG2	2:B:230:TYR:CD2	2.41	0.54
2:A:31:TYR:CG	2:B:46:LEU:HD11	2.42	0.54
2:C:36:ASP:OD1	2:C:38:LYS:HB2	2.08	0.54
2:C:220:GLU:OE1	2:C:220:GLU:HA	2.07	0.54
2:C:49:ARG:HH21	2:C:65:GLU:CD	2.10	0.54
2:B:72:TYR:CE2	2:B:73:PRO:HB3	2.43	0.54
1:E:8:DC:H2"	1:E:9:DC:H6	1.69	0.53
2:A:24:ILE:HG23	2:A:24:ILE:O	2.07	0.53
2:C:188:ASN:HD22	2:C:188:ASN:N	2.06	0.53
2:A:151:TYR:HD1	2:A:151:TYR:H	1.56	0.53
2:A:64:GLU:N	2:A:76:THR:O	2.41	0.53
2:A:233:ILE:HG23	2:A:234:SER:N	2.23	0.53
2:A:237:ARG:O	2:A:240:ILE:HG22	2.09	0.53
2:C:62:ILE:CD1	2:C:80:PRO:HG3	2.39	0.53
2:B:78:TYR:CD2	2:B:86:LYS:HD3	2.44	0.53
2:A:171:GLN:NE2	2:A:202:GLY:CA	2.72	0.53
2:B:100:ASN:ND2	2:B:195:HIS:CD2	2.77	0.52
2:B:119:LYS:O	2:B:120:ASN:HB2	2.09	0.52
2:B:33:LEU:HB2	2:B:162:PRO:CG	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:VAL:CG1	2:A:43:ILE:HD11	2.39	0.52
2:B:192:ILE:HD11	2:B:205:ILE:HB	1.91	0.52
2:C:110:TYR:CD1	2:C:111:THR:HG23	2.44	0.52
2:C:171:GLN:NE2	2:C:172:ASP:N	2.39	0.52
2:C:3:LEU:HD23	2:C:87:ILE:CD1	2.39	0.52
2:C:106:THR:HG22	2:C:182:GLY:HA3	1.91	0.52
2:B:171:GLN:HG3	2:B:172:ASP:N	2.24	0.52
1:E:4:DA:H5'	2:A:119:LYS:HZ2	1.74	0.52
2:C:132:TRP:HB3	2:C:170:LEU:HD11	1.92	0.52
2:A:206:PHE:CD1	2:A:233:ILE:HD12	2.44	0.52
2:B:138:TYR:CD1	2:B:138:TYR:N	2.78	0.52
2:A:4:ARG:NH1	2:A:172:ASP:OD1	2.29	0.52
2:B:241:TYR:CD1	2:B:241:TYR:N	2.78	0.51
2:A:179:ASP:HB2	2:A:215:TYR:OH	2.10	0.51
2:C:86:LYS:HE2	2:C:123:TYR:CE2	2.44	0.51
2:B:229:LYS:O	2:B:230:TYR:HB3	2.11	0.51
2:C:209:GLU:O	2:C:209:GLU:HG3	2.10	0.51
2:B:157:ASN:OD1	2:B:157:ASN:N	2.38	0.51
2:B:20:VAL:HG12	2:B:20:VAL:O	2.09	0.51
2:A:151:TYR:CG	2:A:159:ILE:HG12	2.45	0.51
2:B:94:THR:O	2:B:137:VAL:HA	2.10	0.51
2:A:93:THR:HG22	2:A:136:TYR:HB2	1.93	0.51
2:C:238:ASN:O	2:C:240:ILE:N	2.44	0.51
2:A:171:GLN:HE22	2:A:202:GLY:HA3	1.75	0.51
2:C:216:TRP:HZ3	2:C:219:TYR:CD2	2.28	0.51
2:A:214:ASP:OD2	2:A:236:TYR:OH	2.26	0.51
2:A:121:ILE:HG23	2:A:123:TYR:O	2.10	0.51
2:C:107:LEU:HB2	2:C:189:ILE:HG22	1.93	0.51
2:B:221:ARG:NH1	2:B:221:ARG:CB	2.74	0.51
2:C:197:LYS:HE2	2:C:201:GLU:OE2	2.11	0.51
2:B:25:SER:HB2	2:B:27:GLU:OE2	2.11	0.50
2:C:83:PRO:O	2:C:86:LYS:NZ	2.43	0.50
2:C:92:LYS:HE3	2:C:106:THR:O	2.11	0.50
2:A:39:VAL:HG12	2:A:43:ILE:HD12	1.90	0.50
2:B:189:ILE:HG23	2:B:216:TRP:CZ2	2.46	0.50
2:B:238:ASN:CA	2:B:241:TYR:HE1	2.15	0.50
2:A:39:VAL:O	2:A:43:ILE:HD12	2.12	0.50
2:B:36:ASP:OD1	2:B:38:LYS:N	2.42	0.50
2:B:35:SER:HB3	2:B:140:ARG:NH1	2.27	0.50
2:B:62:ILE:N	2:B:78:TYR:O	2.26	0.50
2:A:102:LYS:HD2	2:A:193:HIS:O	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:171:GLN:CA	2:C:171:GLN:NE2	2.75	0.50
2:B:62:ILE:O	2:B:77:LEU:HA	2.11	0.50
2:B:240:ILE:HG22	2:B:240:ILE:O	2.12	0.50
2:C:11:LEU:CD1	2:C:134:ILE:HD13	2.30	0.49
1:D:9:DC:H42	1:E:2:DG:H1	1.60	0.49
2:B:174:TRP:CD1	2:B:209:GLU:HB2	2.46	0.49
2:A:138:TYR:HE1	2:A:140:ARG:HB3	1.77	0.49
2:C:77:LEU:HD13	2:C:89:ILE:HD12	1.94	0.49
2:B:206:PHE:HE1	2:B:215:TYR:CB	2.26	0.49
2:C:88:ALA:HB2	2:C:128:TYR:CD1	2.48	0.49
2:B:240:ILE:H	2:B:240:ILE:HD12	1.74	0.49
2:A:153:ILE:CG1	2:B:153:ILE:HD13	2.43	0.49
2:C:172:ASP:HB2	2:C:175:VAL:HG23	1.95	0.49
2:C:114:ILE:HD12	2:C:213:LEU:CD2	2.43	0.49
2:C:30:ILE:HD12	2:C:152:ASN:C	2.33	0.49
2:C:95:TYR:CD1	2:C:140:ARG:HG2	2.47	0.49
1:F:4:DA:H2''	1:F:5:DT:O5'	2.13	0.49
2:A:103:ILE:O	2:A:193:HIS:HA	2.13	0.49
2:A:7:LEU:O	2:A:7:LEU:HD12	2.13	0.48
1:F:5:DT:H73	2:C:186:THR:HB	1.95	0.48
2:A:94:THR:HG22	2:A:105:PHE:CZ	2.48	0.48
2:C:215:TYR:CE1	2:C:230:TYR:CE1	3.01	0.48
2:A:231:ASN:O	2:A:232:ASN:HB3	2.12	0.48
2:A:88:ALA:C	2:A:89:ILE:HG12	2.33	0.48
2:C:77:LEU:O	2:C:78:TYR:HB3	2.13	0.48
2:A:171:GLN:HG2	2:A:176:ILE:HG23	1.95	0.48
2:B:163:TYR:N	2:B:163:TYR:CD1	2.81	0.48
2:C:69:GLN:HB2	3:C:762:HOH:O	2.14	0.48
2:B:77:LEU:N	2:B:77:LEU:HD12	2.28	0.48
2:A:19:ASP:O	2:B:25:SER:HB2	2.12	0.48
2:B:233:ILE:HG23	2:B:234:SER:N	2.27	0.48
2:B:49:ARG:NE	2:B:65:GLU:OE1	2.39	0.48
2:C:216:TRP:CZ3	2:C:219:TYR:CD2	3.02	0.48
2:A:179:ASP:OD2	2:A:232:ASN:HB2	2.12	0.48
2:A:31:TYR:CE1	2:A:150:THR:CG2	2.97	0.48
2:B:221:ARG:NH1	2:B:221:ARG:HB3	2.29	0.48
2:B:3:LEU:HD23	2:B:87:ILE:CD1	2.45	0.47
2:B:49:ARG:HB3	2:B:49:ARG:NH1	2.28	0.47
2:C:156:LEU:HA	2:C:156:LEU:HD12	1.73	0.47
2:A:35:SER:HB2	2:A:140:ARG:HD3	1.96	0.47
2:B:233:ILE:CG2	2:B:234:SER:N	2.78	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:239:TRP:C	2:A:241:TYR:H	2.17	0.47
1:D:4:DA:H4'	2:B:120:ASN:CG	2.35	0.47
2:B:174:TRP:CZ3	2:B:208:SER:CA	2.98	0.47
2:A:89:ILE:HD13	2:A:132:TRP:CE3	2.45	0.47
2:A:91:ILE:CD1	2:A:91:ILE:N	2.78	0.47
1:D:4:DA:H2''	1:D:5:DT:O5'	2.15	0.47
2:A:152:ASN:O	2:A:154:ASN:N	2.48	0.47
2:A:21:CYS:N	2:B:24:ILE:O	2.39	0.47
2:B:189:ILE:CG2	2:B:190:GLY:N	2.78	0.46
2:C:3:LEU:CD2	2:C:87:ILE:HD12	2.45	0.46
2:C:60:GLY:O	2:C:79:LYS:HG2	2.15	0.46
1:E:6:DA:H2''	1:E:7:DT:H5'	1.96	0.46
2:C:170:LEU:HG	2:C:171:GLN:N	2.29	0.46
2:A:211:GLU:OE2	2:A:233:ILE:HD11	2.15	0.46
2:B:221:ARG:CG	2:B:221:ARG:NH1	2.77	0.46
2:C:38:LYS:HE2	2:C:38:LYS:HB2	1.76	0.46
2:C:27:GLU:CD	2:C:27:GLU:N	2.68	0.46
2:A:64:GLU:OE1	2:A:123:TYR:OH	2.27	0.46
2:C:82:GLU:N	2:C:83:PRO:CD	2.78	0.46
2:A:233:ILE:CG2	2:A:234:SER:N	2.78	0.46
2:B:155:GLU:O	2:B:158:GLU:HB2	2.15	0.46
2:A:87:ILE:CG1	2:A:130:ALA:HB3	2.46	0.46
2:B:49:ARG:HB2	2:B:75:PHE:CE2	2.51	0.46
2:B:72:TYR:CD2	2:B:73:PRO:HB3	2.51	0.46
2:B:151:TYR:N	2:B:151:TYR:CD1	2.84	0.46
2:A:124:PRO:HD2	2:A:127:GLN:NE2	2.31	0.46
2:B:236:TYR:O	2:B:239:TRP:N	2.49	0.46
2:A:110:TYR:CD1	2:A:111:THR:HG23	2.51	0.46
2:C:75:PHE:HB2	2:C:89:ILE:HB	1.98	0.45
2:C:62:ILE:CG2	2:C:63:VAL:N	2.79	0.45
2:C:114:ILE:HA	2:C:114:ILE:HD13	1.63	0.45
2:B:29:LYS:NZ	2:B:150:THR:CG2	2.80	0.45
2:A:133:ILE:N	2:A:133:ILE:HD13	2.30	0.45
2:B:140:ARG:HG3	2:B:140:ARG:O	2.15	0.45
2:A:22:GLY:O	2:B:24:ILE:HG22	2.16	0.45
2:A:153:ILE:HG21	2:B:153:ILE:HD11	1.99	0.45
1:F:5:DT:C7	2:C:186:THR:HB	2.45	0.45
2:A:89:ILE:CD1	2:A:132:TRP:CE3	2.99	0.45
2:C:86:LYS:O	2:C:129:ILE:HG12	2.16	0.45
2:C:48:SER:O	2:C:52:ILE:HG13	2.15	0.45
2:B:123:TYR:HB2	2:B:128:TYR:CE1	2.51	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:LEU:HD12	2:C:159:ILE:HD12	1.98	0.45
2:C:136:TYR:HA	2:C:167:LYS:O	2.17	0.45
2:A:238:ASN:O	2:A:241:TYR:N	2.46	0.45
2:A:164:LYS:HE3	2:A:164:LYS:HB2	1.47	0.45
2:B:44:PHE:CD2	2:B:93:THR:HG21	2.52	0.45
2:B:8:ILE:HG23	2:B:12:TYR:HE2	1.82	0.45
2:A:110:TYR:CD1	2:A:111:THR:CG2	3.00	0.45
2:B:66:PRO:HB3	2:B:122:VAL:CG2	2.47	0.44
2:A:49:ARG:HG2	2:A:49:ARG:O	2.14	0.44
1:D:4:DA:H5'	2:B:119:LYS:NZ	2.32	0.44
2:B:221:ARG:CB	2:B:221:ARG:CZ	2.96	0.44
2:B:40:LEU:HA	2:B:43:ILE:HD12	1.98	0.44
1:E:6:DA:H2'	1:E:7:DT:H5'	1.94	0.44
2:C:62:ILE:HG22	2:C:63:VAL:N	2.32	0.44
2:B:86:LYS:O	2:B:128:TYR:HA	2.17	0.44
2:C:73:PRO:HG2	2:C:75:PHE:O	2.16	0.44
2:C:136:TYR:CD1	2:C:168:VAL:HG23	2.52	0.44
2:C:51:ILE:H	2:C:51:ILE:HG13	1.57	0.44
2:B:135:GLY:HA3	2:B:169:PHE:CZ	2.52	0.44
2:A:171:GLN:NE2	2:A:202:GLY:HA3	2.32	0.44
2:A:153:ILE:HB	2:B:153:ILE:CD1	2.48	0.44
2:B:137:VAL:O	2:B:166:VAL:HA	2.17	0.44
2:B:139:THR:HB	2:B:164:LYS:HB3	2.00	0.44
2:B:7:LEU:HA	2:B:7:LEU:HD12	1.78	0.44
2:A:31:TYR:CD1	2:A:150:THR:CG2	3.01	0.44
2:C:49:ARG:CB	2:C:50:PRO:CD	2.96	0.44
2:A:233:ILE:CD1	2:A:237:ARG:NH2	2.81	0.43
2:A:171:GLN:CG	2:A:172:ASP:N	2.80	0.43
2:B:107:LEU:HD22	2:B:133:ILE:HD11	2.00	0.43
2:B:229:LYS:HG2	2:B:230:TYR:HD2	1.83	0.43
2:A:95:TYR:O	2:A:96:THR:HG23	2.17	0.43
2:C:170:LEU:O	2:C:171:GLN:HB2	2.18	0.43
2:B:4:ARG:NH1	2:B:172:ASP:OD1	2.48	0.43
2:A:138:TYR:CE1	2:A:140:ARG:HB3	2.53	0.43
2:C:86:LYS:HE2	2:C:123:TYR:CD2	2.53	0.43
2:C:49:ARG:N	2:C:50:PRO:CD	2.80	0.43
2:A:110:TYR:CZ	2:A:187:THR:HG23	2.53	0.43
2:A:93:THR:HA	2:A:136:TYR:O	2.18	0.43
2:C:121:ILE:HG12	2:C:122:VAL:N	2.32	0.43
2:A:132:TRP:O	2:A:133:ILE:HD13	2.18	0.43
2:A:159:ILE:HG22	2:A:160:PRO:N	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:73:PRO:HG3	2:A:88:ALA:CB	2.49	0.43
2:C:82:GLU:O	2:C:84:ASN:N	2.51	0.43
2:A:151:TYR:N	2:A:151:TYR:CD1	2.85	0.43
2:C:187:THR:O	2:C:187:THR:HG22	2.19	0.43
2:B:86:LYS:HE2	2:B:123:TYR:CE2	2.53	0.43
2:B:11:LEU:HD23	2:B:11:LEU:HA	1.84	0.43
2:B:206:PHE:CE1	2:B:215:TYR:CB	3.02	0.43
2:A:3:LEU:C	2:A:3:LEU:HD12	2.36	0.43
2:B:136:TYR:HA	2:B:167:LYS:O	2.19	0.43
2:B:122:VAL:HG12	2:B:123:TYR:CE1	2.52	0.42
2:A:42:THR:CG2	2:B:39:VAL:HG21	2.46	0.42
2:A:205:ILE:HG22	2:A:206:PHE:N	2.34	0.42
2:C:138:TYR:HB3	2:C:166:VAL:HG22	2.02	0.42
2:B:110:TYR:HB3	2:B:189:ILE:HG13	2.01	0.42
2:A:77:LEU:N	2:A:77:LEU:HD12	2.35	0.42
2:B:39:VAL:HG12	2:B:43:ILE:HD11	2.01	0.42
2:A:158:GLU:O	2:A:160:PRO:HD3	2.20	0.42
2:C:221:ARG:HG2	2:C:221:ARG:H	1.46	0.42
2:A:66:PRO:HD3	2:A:74:ASP:O	2.20	0.42
2:B:7:LEU:HD23	2:B:170:LEU:HD22	2.01	0.42
2:A:140:ARG:O	2:A:140:ARG:HG3	2.20	0.42
2:A:171:GLN:NE2	2:A:202:GLY:HA2	2.34	0.42
2:C:179:ASP:N	2:C:179:ASP:OD1	2.51	0.42
2:C:68:GLN:OE1	2:C:71:HIS:CG	2.73	0.42
2:A:189:ILE:HD13	2:A:212:PHE:HE2	1.84	0.42
2:C:24:ILE:HG23	2:C:24:ILE:O	2.18	0.42
1:E:5:DT:C4	1:E:6:DA:N7	2.88	0.42
1:E:1:DG:H2''	1:E:2:DG:C8	2.54	0.42
2:B:81:SER:C	2:B:83:PRO:HD3	2.38	0.42
2:A:105:PHE:HB2	2:A:191:SER:CB	2.47	0.42
2:B:49:ARG:N	2:B:50:PRO:HD2	2.35	0.42
1:E:4:DA:H5'	2:A:119:LYS:HZ3	1.83	0.41
2:C:203:LYS:HA	2:C:203:LYS:HD2	1.82	0.41
2:B:30:ILE:CD1	2:B:156:LEU:HD21	2.50	0.41
2:C:75:PHE:HE2	2:C:91:ILE:HD12	1.84	0.41
2:B:218:ASN:OD1	2:B:218:ASN:N	2.53	0.41
2:A:233:ILE:HD11	2:A:237:ARG:NH2	2.35	0.41
2:C:77:LEU:CD1	2:C:89:ILE:HD12	2.50	0.41
2:B:8:ILE:CG2	2:B:12:TYR:CE2	2.97	0.41
2:A:92:LYS:O	2:A:135:GLY:HA2	2.21	0.41
2:A:159:ILE:HA	2:A:160:PRO:HD3	1.86	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:110:TYR:CE1	2:A:187:THR:HG23	2.56	0.41
2:C:235:GLU:O	2:C:239:TRP:HB2	2.21	0.41
2:B:100:ASN:HD21	2:B:195:HIS:CD2	2.33	0.41
2:C:240:ILE:O	2:C:240:ILE:HG22	2.20	0.41
2:C:68:GLN:HB2	2:C:71:HIS:ND1	2.35	0.41
2:A:23:ILE:O	2:A:30:ILE:HG23	2.21	0.41
2:C:40:LEU:HD23	2:C:40:LEU:HA	1.82	0.41
2:A:239:TRP:C	2:A:241:TYR:N	2.73	0.41
1:E:2:DG:C6	1:E:3:DG:C6	3.09	0.41
2:C:90:ASP:HB3	2:C:133:ILE:CD1	2.51	0.41
2:A:179:ASP:HB2	2:A:232:ASN:HA	2.03	0.41
2:B:40:LEU:HD23	2:B:40:LEU:HA	1.76	0.41
2:B:8:ILE:O	2:B:12:TYR:CD2	2.74	0.41
2:A:153:ILE:HG12	2:A:153:ILE:O	2.19	0.41
2:B:57:GLU:C	2:B:59:HIS:H	2.24	0.41
2:C:24:ILE:HA	2:C:29:LYS:O	2.21	0.41
2:C:117:ASN:O	2:C:117:ASN:OD1	2.39	0.41
2:C:187:THR:O	2:C:187:THR:CG2	2.70	0.40
2:A:204:GLY:HA3	3:A:767:HOH:O	2.20	0.40
2:B:8:ILE:HG23	2:B:12:TYR:CE2	2.55	0.40
2:C:61:TYR:CD1	2:C:79:LYS:HG3	2.56	0.40
2:C:11:LEU:HD23	2:C:11:LEU:HA	1.78	0.40
2:A:189:ILE:HD13	2:A:212:PHE:CE2	2.56	0.40
2:C:77:LEU:HD13	2:C:89:ILE:CD1	2.50	0.40
2:A:77:LEU:N	2:A:77:LEU:CD1	2.84	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
2	A	238/244 (98%)	190 (80%)	34 (14%)	14 (6%)	2 11

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	238/244 (98%)	191 (80%)	40 (17%)	7 (3%)	6	29
2	C	238/244 (98%)	190 (80%)	31 (13%)	17 (7%)	1	7
All	All	714/732 (98%)	571 (80%)	105 (15%)	38 (5%)	2	14

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	99	GLU
2	A	101	GLU
2	A	144	ARG
2	A	151	TYR
2	A	153	ILE
2	B	15	ASN
2	B	144	ARG
2	B	145	LYS
2	C	13	ASP
2	C	83	PRO
2	C	99	GLU
2	C	117	ASN
2	C	142	ALA
2	C	143	THR
2	C	148	LEU
2	A	15	ASN
2	A	16	GLN
2	A	100	ASN
2	A	196	TYR
2	A	237	ARG
2	B	13	ASP
2	B	35	SER
2	B	125	PHE
2	B	148	LEU
2	C	184	GLY
2	C	227	ASN
2	C	239	TRP
2	A	142	ALA
2	A	143	THR
2	C	14	GLU
2	C	125	PHE
2	C	203	LYS
2	C	228	ASP
2	C	191	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	13	ASP
2	A	141	VAL
2	C	82	GLU
2	C	28	GLY

### 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	
2	A	217/220 (99%)	168 (77%)	49 (23%)	1	5
2	B	217/220 (99%)	161 (74%)	56 (26%)	0	3
2	C	217/220 (99%)	167 (77%)	50 (23%)	1	5
All	All	651/660 (99%)	496 (76%)	155 (24%)	1	4

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	7	LEU
2	A	11	LEU
2	A	16	GLN
2	A	17	LYS
2	A	19	ASP
2	A	20	VAL
2	A	23	ILE
2	A	29	LYS
2	A	38	LYS
2	A	41	SER
2	A	45	GLU
2	A	67	LYS
2	A	69	GLN
2	A	71	HIS
2	A	74	ASP
2	A	81	SER
2	A	84	ASN
2	A	87	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	89	ILE
2	A	90	ASP
2	A	92	LYS
2	A	99	GLU
2	A	100	ASN
2	A	101	GLU
2	A	103	ILE
2	A	107	LEU
2	A	114	ILE
2	A	115	ARG
2	A	140	ARG
2	A	144	ARG
2	A	146	SER
2	A	147	SER
2	A	148	LEU
2	A	152	ASN
2	A	153	ILE
2	A	158	GLU
2	A	164	LYS
2	A	188	ASN
2	A	191	SER
2	A	212	PHE
2	A	214	ASP
2	A	221	ARG
2	A	223	SER
2	A	227	ASN
2	A	234	SER
2	A	237	ARG
2	A	238	ASN
2	A	240	ILE
2	A	241	TYR
2	B	2	SER
2	B	4	ARG
2	B	9	ASN
2	B	15	ASN
2	B	17	LYS
2	B	21	CYS
2	B	23	ILE
2	B	27	GLU
2	B	29	LYS
2	B	30	ILE
2	B	41	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	46	LEU
2	B	48	SER
2	B	49	ARG
2	B	72	TYR
2	B	73	PRO
2	B	81	SER
2	B	82	GLU
2	B	84	ASN
2	B	91	ILE
2	B	92	LYS
2	B	94	THR
2	B	97	ASN
2	B	103	ILE
2	B	104	LYS
2	B	106	THR
2	B	114	ILE
2	B	126	ASP
2	B	129	ILE
2	B	137	VAL
2	B	140	ARG
2	B	144	ARG
2	B	146	SER
2	B	148	LEU
2	B	150	THR
2	B	152	ASN
2	B	155	GLU
2	B	157	ASN
2	B	164	LYS
2	B	167	LYS
2	B	183	SER
2	B	188	ASN
2	B	191	SER
2	B	192	ILE
2	B	197	LYS
2	B	203	LYS
2	B	205	ILE
2	B	210	ASP
2	B	212	PHE
2	B	218	ASN
2	B	221	ARG
2	B	223	SER
2	B	228	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	237	ARG
2	B	240	ILE
2	B	241	TYR
2	C	2	SER
2	C	9	ASN
2	C	12	TYR
2	C	14	GLU
2	C	15	ASN
2	C	21	CYS
2	C	27	GLU
2	C	38	LYS
2	C	41	SER
2	C	42	THR
2	C	46	LEU
2	C	48	SER
2	C	49	ARG
2	C	68	GLN
2	C	70	ASN
2	C	71	HIS
2	C	82	GLU
2	C	90	ASP
2	C	92	LYS
2	C	94	THR
2	C	99	GLU
2	C	100	ASN
2	C	104	LYS
2	C	115	ARG
2	C	134	ILE
2	C	140	ARG
2	C	143	THR
2	C	144	ARG
2	C	148	LEU
2	C	149	LYS
2	C	151	TYR
2	C	153	ILE
2	C	157	ASN
2	C	158	GLU
2	C	168	VAL
2	C	171	GLN
2	C	185	ASN
2	C	188	ASN
2	C	192	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	203	LYS
2	C	205	ILE
2	C	210	ASP
2	C	221	ARG
2	C	223	SER
2	C	224	GLN
2	C	225	LEU
2	C	226	ARG
2	C	234	SER
2	C	238	ASN
2	C	241	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	69	GLN
2	A	127	GLN
2	B	84	ASN
2	B	100	ASN
2	B	195	HIS
2	B	231	ASN
2	B	238	ASN
2	C	171	GLN
2	C	185	ASN
2	C	188	ASN
2	C	193	HIS
2	C	238	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.