



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:01 AM UTC

PDB ID : 1IC8 / pdb_00001ic8
Title : HEPATOCYTE NUCLEAR FACTOR 1A BOUND TO DNA : MODY3 GENE PRODUCT
Authors : Chi, Y.-I.; Frantz, J.D.; Oh, B.-C.; Hansen, L.; Dhe-Paganon, S.; Shoelson, S.E.
Deposited on : 2001-03-30
Resolution : 2.60 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

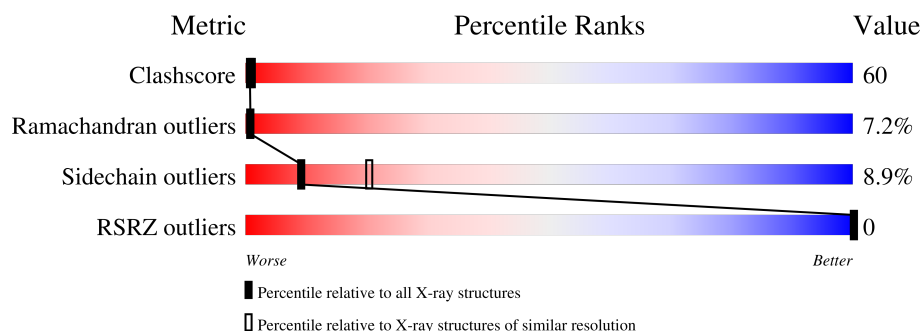
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	E	21	19% 76% 5%
2	F	21	19% 81%
3	A	194	16% 59% 10% • 12%
3	B	194	25% 56% 8% • 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3826 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 5'-D(*CP*TP*TP*GP*GP*TP*TP*AP*AP*TP*AP*AP*TP*TP*CP*AP*CP*CP*AP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	21	Total	C	N	O	P	0	0	0
			426	206	76	124	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	21	Total	C	N	O	P	0	0	0
			429	207	78	124	20			

- Molecule 3 is a protein called HEPATOCYTE NUCLEAR FACTOR 1-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	170	Total	C	N	O	S	0	0	0
			1399	868	266	261	4			
3	B	173	Total	C	N	O	S	0	0	0
			1433	892	272	265	4			

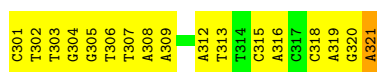
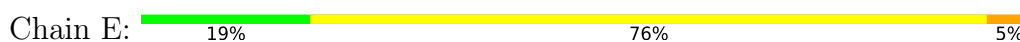
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	18	Total	O	0	0
			18	18		
4	F	16	Total	O	0	0
			16	16		
4	A	45	Total	O	0	0
			45	45		
4	B	60	Total	O	0	0
			60	60		

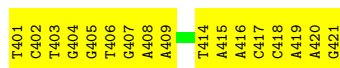
3 Residue-property plots

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.

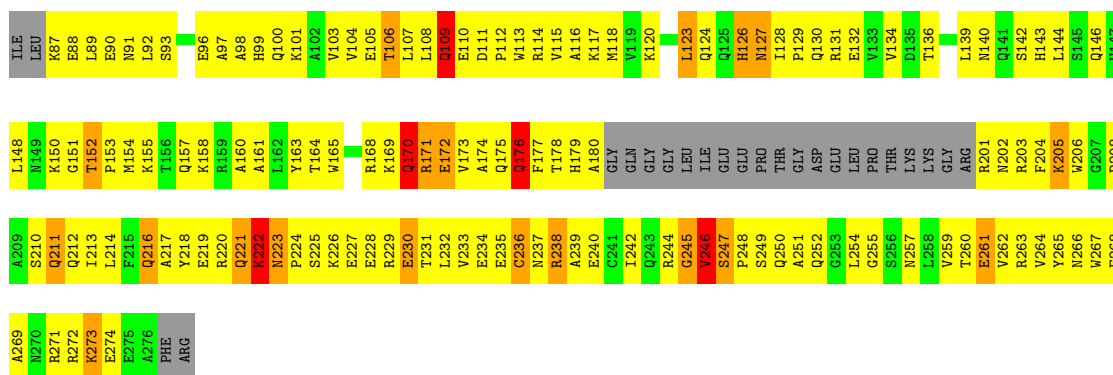
- Molecule 1: 5'-D(*CP*TP*TP*GP*GP*TP*TP*AP*AP*TP*AP*AP*TP*TP*CP*AP*CP*CP*AP*GP*A)-3'



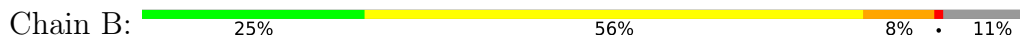
- Molecule 2: 5'-D(*TP*CP*TP*GP*GP*TP*GP*AP*AP*TP*TP*AP*TP*TP*AP*AP*CP*CP*AP*AP*G)-3'



- Molecule 3: HEPATOCYTE NUCLEAR FACTOR 1-ALPHA



- Molecule 3: HEPATOCYTE NUCLEAR FACTOR 1-ALPHA



T152	F153	M154	K155	T156	Q157	K158	R159	A160	A161	L162	Y163	T164	M165	Y166	V167	R168	K169	Q170	R171	E172	V173	A174	Q175	Q176	F177	T178	H179	ALA	GLY	GLN	GLY	GLY	LEU	ILE	GLU	GLU	PRO	PRO	THR	GLY	ASP	GLU	LEU	GLU	LEU	PRO	THR	LYS	LYS	GLY	GLY	ARG	R201	N202	R203	F204	K205	W206	A209	S210	Q211	Q212
I213	L214	F215	Q216	A217	Y218	Q221	K222	N223	P224	S225	K226	E227	E228	R229	E230	T231	L232	V233	E234	E235	C236	N237	R238	A239	E240	C241	R244	G245	V246	S247	P248	A251	Q252	G253	S256	N257	L258	V259	T260	E261	V262	R263	V264	Y265	N266	N270	R271	R272	K273	E274	F277	R278										

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	50.39Å 50.39Å 207.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.40 – 2.60 29.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.40-2.60) 93.5 (29.40-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.254 , 0.312 0.262 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3826	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.89% 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

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	E	0.37	0/477	0.82	1/734 (0.1%)
2	F	0.35	0/481	0.80	0/741
3	A	0.58	0/1426	1.08	12/1923 (0.6%)
3	B	0.56	0/1461	1.05	9/1968 (0.5%)
All	All	0.52	0/3845	1.00	22/5366 (0.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	171	ARG	N-CA-C	-7.90	103.53	113.02
3	B	90	GLU	N-CA-C	-7.00	104.00	114.64
3	A	152	THR	CA-C-N	6.73	127.09	119.83
3	A	152	THR	C-N-CA	6.73	127.09	119.83
3	B	227	GLU	N-CA-C	-6.14	104.70	111.82
3	A	176	GLN	N-CA-C	-6.14	105.07	113.30
3	B	109	GLN	N-CA-C	-5.99	106.01	113.55
3	B	231	THR	N-CA-C	-5.86	104.30	112.45
3	B	173	VAL	N-CA-C	-5.86	105.38	113.00
1	E	321	DA	C2'-C3'-O3'	-5.70	102.95	111.50
3	A	109	GLN	N-CA-C	-5.62	107.05	114.31
3	A	238	ARG	N-CA-C	-5.27	105.53	111.28
3	A	174	ALA	N-CA-C	-5.26	105.97	112.38
3	A	171	ARG	NE-CZ-NH2	5.23	123.91	119.20
3	B	137	THR	N-CA-C	-5.20	106.33	113.30
3	A	106	THR	N-CA-C	-5.18	106.11	112.90
3	A	171	ARG	O-C-N	5.18	129.07	122.39
3	B	248	PRO	CB-CA-C	-5.16	103.05	111.56
3	B	156	THR	N-CA-C	5.14	117.29	111.02
3	B	104	VAL	N-CA-C	-5.12	105.39	110.62
3	A	236	CYS	N-CA-C	-5.06	104.76	112.04
3	A	230	GLU	N-CA-C	-5.04	105.91	111.71

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	E	426	0	240	44	0
2	F	429	0	240	48	0
3	A	1399	0	1378	174	0
3	B	1433	0	1417	162	0
4	A	45	0	0	8	0
4	B	60	0	0	4	0
4	E	18	0	0	0	0
4	F	16	0	0	2	0
All	All	3826	0	3275	410	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 60.

All (410) 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)
2:F:404:DG:H2''	2:F:405:DG:H5''	1.12	1.08
3:A:127:ASN:HB3	3:A:257:ASN:ND2	1.72	1.03
3:A:176:GLN:HG2	3:A:246:VAL:HG11	1.36	1.03
3:A:222:LYS:H	3:A:222:LYS:HD3	1.20	1.03
1:E:304:DG:H2''	1:E:305:DG:H5''	1.41	1.00
2:F:404:DG:C2'	2:F:405:DG:H5''	1.94	0.97
1:E:304:DG:H2''	1:E:305:DG:C5'	1.95	0.97
2:F:405:DG:H2''	2:F:406:DT:H5'	1.46	0.95
3:A:237:ASN:HD21	3:A:259:VAL:H	1.11	0.94
2:F:401:DT:H1'	2:F:402:DC:O5'	1.68	0.94
3:B:225:SER:OG	3:B:228:GLU:HB2	1.71	0.91
2:F:404:DG:H2''	2:F:405:DG:C5'	2.00	0.90
3:A:248:PRO:HG2	3:A:251:ALA:HB2	1.51	0.90
3:A:247:SER:H	3:A:248:PRO:CD	1.87	0.87
3:B:93:SER:HB3	3:B:96:GLU:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:THR:OG1	3:A:262:VAL:HG22	1.75	0.86
3:B:171:ARG:HG3	3:B:172:GLU:N	1.90	0.85
3:B:154:MET:HE2	3:B:159:ARG:HA	1.60	0.82
3:A:232:LEU:HA	3:A:235:GLU:HB3	1.61	0.81
3:A:216:GLN:HB3	3:A:220:ARG:HH12	1.47	0.80
3:A:252:GLN:HA	4:A:1104:HOH:O	1.82	0.79
3:B:140:ASN:ND2	3:B:143:HIS:H	1.80	0.79
3:A:93:SER:HB3	3:A:96:GLU:HB3	1.65	0.79
3:A:223:ASN:HA	4:A:1082:HOH:O	1.82	0.78
3:B:127:ASN:HB3	3:B:257:ASN:OD1	1.84	0.78
3:A:127:ASN:HB3	3:A:257:ASN:HD21	1.46	0.78
3:A:87:LYS:HE2	3:A:87:LYS:HA	1.65	0.77
3:A:223:ASN:HD21	3:A:225:SER:HB3	1.50	0.77
1:E:304:DG:C2'	1:E:305:DG:H5''	2.15	0.77
2:F:401:DT:H2''	2:F:402:DC:OP2	1.83	0.77
3:B:121:SER:O	3:B:125:GLN:HG2	1.84	0.76
3:B:172:GLU:O	3:B:172:GLU:HG2	1.86	0.75
3:B:169:LYS:C	3:B:171:ARG:H	1.95	0.75
3:A:127:ASN:HB3	3:A:257:ASN:HD22	1.52	0.74
3:A:140:ASN:ND2	3:A:143:HIS:H	1.84	0.74
3:A:221:GLN:OE1	3:A:223:ASN:HB3	1.87	0.74
3:B:237:ASN:ND2	3:B:259:VAL:HB	2.02	0.74
1:E:312:DA:H2''	1:E:313:DT:H5'	1.69	0.73
3:B:216:GLN:C	3:B:218:TYR:H	1.96	0.73
1:E:320:DG:H2''	1:E:321:DA:C8	2.24	0.73
3:A:134:VAL:HG13	3:A:139:LEU:O	1.89	0.73
3:A:217:ALA:HB2	3:A:232:LEU:HD11	1.69	0.73
2:F:417:DC:H4'	2:F:417:DC:OP1	1.86	0.73
3:B:140:ASN:HD22	3:B:143:HIS:HB2	1.52	0.73
3:A:151:GLY:HA3	3:B:277:PHE:HB2	1.71	0.72
3:A:178:THR:C	3:A:180:ALA:H	1.97	0.72
3:B:251:ALA:O	3:B:253:GLY:N	2.22	0.72
3:B:271:ARG:O	3:B:274:GLU:HB3	1.89	0.72
3:B:240:GLU:O	3:B:244:ARG:HG2	1.89	0.72
3:A:169:LYS:C	3:A:171:ARG:H	1.97	0.71
2:F:401:DT:H1'	2:F:402:DC:P	2.31	0.71
3:A:260:THR:O	3:A:264:VAL:HG23	1.91	0.71
3:A:272:ARG:HG3	3:A:272:ARG:HH11	1.55	0.70
3:B:93:SER:HB3	3:B:96:GLU:CB	2.20	0.70
3:A:222:LYS:HD3	3:A:222:LYS:N	2.00	0.70
2:F:402:DC:H2'	2:F:403:DT:H71	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:225:SER:O	3:B:228:GLU:N	2.22	0.69
1:E:304:DG:N7	3:A:273:LYS:NZ	2.37	0.69
3:B:107:LEU:HD22	3:B:115:VAL:HG13	1.73	0.69
3:A:247:SER:H	3:A:248:PRO:HD3	1.57	0.69
2:F:418:DC:H2''	2:F:419:DA:C8	2.27	0.69
3:A:238:ARG:O	3:A:242:ILE:HG13	1.93	0.69
3:B:247:SER:N	3:B:248:PRO:CD	2.56	0.68
3:A:236:CYS:HB3	3:A:259:VAL:HG21	1.75	0.68
3:B:101:LYS:O	3:B:105:GLU:HB2	1.94	0.68
3:B:246:VAL:HG23	3:B:246:VAL:O	1.94	0.68
3:B:140:ASN:HD21	3:B:142:SER:HB3	1.58	0.67
3:B:216:GLN:O	3:B:218:TYR:N	2.28	0.67
3:A:269:ALA:O	3:A:272:ARG:HB2	1.94	0.67
3:B:248:PRO:HB2	3:B:251:ALA:HB2	1.77	0.67
3:B:240:GLU:OE1	3:B:244:ARG:NH2	2.28	0.66
3:A:261:GLU:N	3:A:261:GLU:CD	2.52	0.66
2:F:408:DA:H2''	2:F:409:DA:H5'	1.75	0.66
3:A:261:GLU:C	3:A:263:ARG:H	2.02	0.66
3:B:172:GLU:HA	3:B:175:GLN:HG3	1.78	0.66
3:A:127:ASN:HD21	3:A:205:LYS:HD2	1.61	0.66
1:E:304:DG:H2''	1:E:305:DG:H5'	1.75	0.66
1:E:320:DG:H2''	1:E:321:DA:N7	2.11	0.66
3:A:113:TRP:O	3:A:117:LYS:HG2	1.96	0.66
3:A:229:ARG:O	3:A:233:VAL:HG23	1.97	0.65
3:A:210:SER:O	3:A:213:ILE:HG22	1.96	0.65
3:B:164:THR:HG22	3:B:168:ARG:HD2	1.78	0.65
1:E:308:DA:H2''	1:E:309:DA:C5'	2.27	0.65
3:B:140:ASN:HD22	3:B:143:HIS:H	1.43	0.65
2:F:416:DA:H2'	2:F:417:DC:C6	2.32	0.65
3:A:131:ARG:HG2	4:A:1079:HOH:O	1.96	0.65
3:A:206:TRP:CE3	3:A:214:LEU:HD11	2.31	0.65
3:A:247:SER:N	3:A:248:PRO:CD	2.59	0.64
1:E:315:DC:C2'	1:E:316:DA:H5''	2.28	0.64
1:E:315:DC:H42	2:F:407:DG:H1	1.45	0.64
2:F:408:DA:H3'	4:F:1030:HOH:O	1.96	0.64
3:A:237:ASN:HD21	3:A:259:VAL:N	1.89	0.64
2:F:405:DG:H2''	2:F:406:DT:C5'	2.22	0.64
3:A:140:ASN:HD22	3:A:143:HIS:H	1.46	0.64
3:A:90:GLU:O	3:A:92:LEU:N	2.28	0.63
3:A:211:GLN:HA	3:A:214:LEU:HD12	1.79	0.63
3:B:154:MET:HE2	3:B:159:ARG:CA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:97:ALA:O	3:A:101:LYS:HG2	1.99	0.63
3:A:170:GLN:NE2	3:A:170:GLN:N	2.46	0.63
3:A:225:SER:C	3:A:227:GLU:H	2.06	0.63
3:B:247:SER:N	3:B:248:PRO:HD3	2.14	0.63
3:A:127:ASN:ND2	3:A:205:LYS:HB3	2.14	0.63
1:E:315:DC:N3	2:F:407:DG:N2	2.40	0.63
3:A:240:GLU:OE1	3:A:244:ARG:NH2	2.32	0.62
1:E:308:DA:H1'	1:E:309:DA:H5''	1.80	0.62
3:A:229:ARG:HG2	3:A:229:ARG:HH11	1.64	0.62
3:B:157:GLN:O	3:B:160:ALA:HB3	2.00	0.62
2:F:403:DT:H2''	2:F:404:DG:C8	2.34	0.62
3:A:170:GLN:C	3:A:172:GLU:H	2.05	0.62
3:B:238:ARG:HG2	3:B:238:ARG:HH11	1.64	0.62
1:E:315:DC:H2''	1:E:316:DA:H5''	1.80	0.62
3:A:140:ASN:HD22	3:A:143:HIS:HB2	1.65	0.61
2:F:414:DT:H5'	2:F:414:DT:H6	1.65	0.61
3:B:246:VAL:C	3:B:248:PRO:HD2	2.26	0.61
2:F:418:DC:H2''	2:F:419:DA:N7	2.16	0.60
3:B:172:GLU:HB2	3:B:175:GLN:OE1	2.01	0.60
2:F:421:DG:H5'	4:F:1131:HOH:O	2.01	0.60
3:B:129:PRO:CD	3:B:202:ASN:HD21	2.14	0.60
3:B:260:THR:OG1	3:B:263:ARG:HG2	2.01	0.60
3:A:272:ARG:C	3:A:274:GLU:H	2.10	0.60
1:E:305:DG:O6	3:A:273:LYS:HE3	2.02	0.60
3:B:131:ARG:HH21	3:B:132:GLU:HA	1.66	0.60
3:B:171:ARG:CG	3:B:172:GLU:N	2.65	0.59
3:B:248:PRO:HB2	3:B:251:ALA:CB	2.32	0.59
3:A:263:ARG:HG2	3:A:263:ARG:HH11	1.66	0.59
3:A:272:ARG:HG3	3:A:272:ARG:NH1	2.15	0.59
2:F:401:DT:C1'	2:F:402:DC:O5'	2.48	0.59
2:F:406:DT:OP1	3:A:155:LYS:HB2	2.02	0.59
2:F:401:DT:C2'	2:F:402:DC:OP2	2.51	0.59
3:A:146:GLN:O	3:A:150:LYS:O	2.21	0.59
3:A:234:GLU:O	3:A:238:ARG:HG3	2.03	0.59
3:B:177:PHE:C	3:B:179:HIS:H	2.11	0.59
3:A:225:SER:OG	3:A:228:GLU:HB2	2.02	0.58
3:B:169:LYS:O	3:B:171:ARG:N	2.36	0.58
1:E:308:DA:H2''	1:E:309:DA:H5''	1.85	0.58
3:B:204:PHE:HD1	3:B:257:ASN:HA	1.68	0.58
3:B:274:GLU:HB2	4:B:1101:HOH:O	2.01	0.58
3:A:178:THR:O	3:A:180:ALA:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:169:LYS:O	3:A:171:ARG:N	2.37	0.58
1:E:302:DT:H2''	1:E:303:DT:C6	2.39	0.58
3:A:224:PRO:HD3	3:A:272:ARG:NH2	2.19	0.58
3:B:246:VAL:C	3:B:248:PRO:CD	2.77	0.58
2:F:408:DA:H1'	2:F:409:DA:H5''	1.86	0.58
3:B:233:VAL:HG13	3:B:234:GLU:N	2.18	0.58
3:B:172:GLU:HB2	3:B:175:GLN:CD	2.30	0.57
3:B:234:GLU:O	3:B:238:ARG:HG3	2.03	0.57
3:B:171:ARG:HG3	3:B:172:GLU:H	1.66	0.57
3:B:223:ASN:HD21	3:B:225:SER:CB	2.16	0.57
3:B:245:GLY:O	3:B:246:VAL:C	2.48	0.57
3:B:261:GLU:HG3	3:B:262:VAL:N	2.19	0.57
1:E:301:DC:H2'	1:E:302:DT:C6	2.39	0.57
3:B:113:TRP:CH2	3:B:117:LYS:HD2	2.40	0.57
3:A:163:TYR:N	3:A:163:TYR:CD1	2.72	0.57
3:A:247:SER:H	3:A:248:PRO:HD2	1.67	0.57
3:A:176:GLN:HG2	3:A:246:VAL:CG1	2.25	0.57
1:E:315:DC:H1'	1:E:316:DA:H5''	1.86	0.57
3:A:144:LEU:HD12	3:A:148:LEU:HD13	1.85	0.57
3:B:88:GLU:CG	3:B:91:ASN:HB2	2.35	0.57
3:A:248:PRO:C	3:A:250:GLN:N	2.61	0.56
3:B:88:GLU:O	3:B:91:ASN:HB2	2.05	0.56
3:A:158:LYS:O	3:A:161:ALA:N	2.38	0.56
3:B:115:VAL:O	3:B:118:MET:HB2	2.06	0.56
3:A:93:SER:CB	3:A:96:GLU:HB3	2.35	0.56
3:A:230:GLU:HA	3:A:233:VAL:HG23	1.87	0.56
3:B:223:ASN:HD21	3:B:225:SER:HB3	1.70	0.56
1:E:308:DA:C2'	1:E:309:DA:H5''	2.35	0.56
3:A:248:PRO:C	3:A:250:GLN:H	2.14	0.56
3:B:261:GLU:O	3:B:264:VAL:HG22	2.06	0.55
3:B:241:CYS:HB3	3:B:247:SER:HA	1.89	0.55
3:A:163:TYR:N	3:A:163:TYR:HD1	2.04	0.55
3:A:230:GLU:HA	3:A:233:VAL:CG2	2.36	0.55
3:B:164:THR:HG22	3:B:168:ARG:CD	2.36	0.55
2:F:415:DA:H2''	2:F:416:DA:O5'	2.06	0.54
3:A:169:LYS:C	3:A:171:ARG:N	2.66	0.54
1:E:321:DA:C2	2:F:401:DT:C7	2.91	0.54
3:B:100:GLN:O	3:B:103:VAL:HG22	2.07	0.54
3:A:146:GLN:C	3:A:152:THR:HG1	2.14	0.54
3:A:204:PHE:CG	3:A:263:ARG:HD3	2.42	0.54
3:A:178:THR:C	3:A:180:ALA:N	2.64	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:88:GLU:HG3	3:B:91:ASN:HB2	1.90	0.54
3:B:154:MET:HE3	3:B:158:LYS:HB3	1.90	0.54
3:B:216:GLN:C	3:B:218:TYR:N	2.56	0.54
1:E:302:DT:H2''	1:E:303:DT:H71	1.90	0.54
3:B:169:LYS:C	3:B:171:ARG:N	2.64	0.54
3:B:176:GLN:HB2	3:B:246:VAL:HG11	1.90	0.54
3:B:209:ALA:HA	3:B:212:GLN:CD	2.32	0.54
3:A:267:TRP:O	3:A:271:ARG:HG2	2.09	0.53
3:B:176:GLN:NE2	3:B:246:VAL:HG21	2.23	0.53
3:B:221:GLN:C	3:B:223:ASN:H	2.16	0.53
2:F:414:DT:H73	3:B:146:GLN:HE22	1.73	0.53
3:A:216:GLN:O	3:A:217:ALA:C	2.51	0.53
3:B:176:GLN:CD	3:B:246:VAL:HG21	2.33	0.53
3:A:227:GLU:C	3:A:229:ARG:H	2.17	0.53
3:B:163:TYR:N	3:B:163:TYR:CD1	2.76	0.53
3:B:229:ARG:HH11	3:B:265:TYR:HB2	1.74	0.52
3:B:278:ARG:HE	3:B:278:ARG:HA	1.73	0.52
1:E:319:DA:H2''	1:E:320:DG:C8	2.43	0.52
3:A:93:SER:HB3	3:A:96:GLU:CB	2.38	0.52
3:B:206:TRP:HB3	3:B:211:GLN:CG	2.39	0.52
3:A:260:THR:OG1	3:A:263:ARG:HG3	2.10	0.52
2:F:416:DA:C2'	2:F:417:DC:C6	2.93	0.52
3:A:230:GLU:C	3:A:232:LEU:H	2.18	0.52
3:A:208:PRO:O	3:A:212:GLN:HG3	2.10	0.52
3:A:221:GLN:C	3:A:223:ASN:H	2.16	0.52
3:A:210:SER:O	3:A:214:LEU:HG	2.09	0.52
3:B:206:TRP:O	3:B:211:GLN:NE2	2.43	0.52
2:F:420:DA:H2''	2:F:421:DG:C8	2.45	0.51
3:A:206:TRP:CZ3	3:A:214:LEU:HD11	2.45	0.51
3:A:107:LEU:HD22	3:A:115:VAL:HG13	1.91	0.51
3:A:230:GLU:C	3:A:232:LEU:N	2.67	0.51
3:B:221:GLN:O	3:B:223:ASN:N	2.44	0.51
3:B:252:GLN:HG3	3:B:258:LEU:HD11	1.91	0.51
3:B:96:GLU:O	3:B:100:GLN:HG3	2.11	0.51
3:B:230:GLU:C	3:B:233:VAL:HG12	2.36	0.51
3:A:213:ILE:O	3:A:216:GLN:HB2	2.11	0.51
3:B:238:ARG:HG2	3:B:238:ARG:NH1	2.26	0.51
3:A:90:GLU:C	3:A:92:LEU:H	2.19	0.51
3:A:126:HIS:O	3:A:127:ASN:C	2.54	0.51
3:A:225:SER:C	3:A:227:GLU:N	2.69	0.51
3:B:230:GLU:HA	3:B:233:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:100:GLN:O	3:A:103:VAL:HB	2.11	0.50
3:A:221:GLN:O	3:A:223:ASN:N	2.44	0.50
3:A:248:PRO:O	3:A:250:GLN:N	2.44	0.50
1:E:316:DA:H62	3:B:270:ASN:HD21	1.60	0.50
3:A:154:MET:HG2	3:A:158:LYS:HB2	1.93	0.50
3:B:90:GLU:OE1	3:B:90:GLU:HA	2.11	0.50
3:B:102:ALA:O	3:B:105:GLU:HB3	2.12	0.50
3:B:120:LYS:O	3:B:124:GLN:HG3	2.11	0.50
3:B:229:ARG:NH1	3:B:265:TYR:HB2	2.27	0.50
2:F:401:DT:C1'	2:F:402:DC:P	2.95	0.50
3:A:111:ASP:HB3	3:A:114:ARG:HD2	1.94	0.50
3:B:178:THR:O	3:B:179:HIS:C	2.55	0.50
3:A:203:ARG:HD3	4:A:1010:HOH:O	2.12	0.50
2:F:416:DA:H2''	2:F:417:DC:O4'	2.11	0.50
3:A:271:ARG:O	3:A:274:GLU:HB2	2.12	0.50
3:A:214:LEU:HB3	3:A:267:TRP:CE3	2.47	0.49
3:A:236:CYS:CB	3:A:259:VAL:HG21	2.42	0.49
3:A:204:PHE:CD2	3:A:263:ARG:HD3	2.46	0.49
3:A:126:HIS:CE1	3:A:244:ARG:HD3	2.48	0.49
3:B:171:ARG:C	3:B:173:VAL:H	2.19	0.49
3:A:233:VAL:CG2	3:A:261:GLU:OE2	2.61	0.49
1:E:303:DT:H2''	1:E:304:DG:C8	2.48	0.49
1:E:318:DC:H2''	1:E:319:DA:C8	2.48	0.49
3:B:229:ARG:C	3:B:231:THR:H	2.21	0.49
3:A:99:HIS:O	3:A:103:VAL:HG23	2.13	0.49
3:A:272:ARG:O	3:A:274:GLU:N	2.46	0.49
2:F:405:DG:C2'	2:F:406:DT:H5'	2.33	0.48
3:A:104:VAL:O	3:A:108:LEU:HG	2.13	0.48
3:A:254:LEU:O	3:A:255:GLY:C	2.54	0.48
3:B:158:LYS:C	3:B:160:ALA:N	2.70	0.48
3:B:225:SER:C	3:B:227:GLU:N	2.68	0.48
2:F:405:DG:H5'	3:A:153:PRO:HB2	1.95	0.48
3:A:268:PHE:O	3:A:269:ALA:C	2.55	0.48
3:B:103:VAL:HG23	3:B:104:VAL:N	2.28	0.48
3:B:104:VAL:HG23	3:B:105:GLU:N	2.28	0.48
3:A:168:ARG:HD3	3:A:171:ARG:NH2	2.29	0.48
1:E:312:DA:H1'	1:E:313:DT:H5''	1.95	0.48
3:A:205:LYS:HD3	3:A:206:TRP:N	2.28	0.48
3:A:217:ALA:O	3:A:221:GLN:N	2.32	0.48
1:E:308:DA:C1'	1:E:309:DA:H5''	2.43	0.47
3:A:93:SER:O	3:A:97:ALA:N	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:176:GLN:CB	3:B:246:VAL:HG11	2.44	0.47
3:A:92:LEU:HD23	3:A:92:LEU:C	2.39	0.47
1:E:308:DA:H2''	1:E:309:DA:H5'	1.97	0.47
2:F:405:DG:O6	3:B:273:LYS:NZ	2.38	0.47
3:A:164:THR:O	3:A:165:TRP:C	2.58	0.47
3:A:272:ARG:C	3:A:274:GLU:N	2.71	0.47
1:E:302:DT:C2'	1:E:303:DT:H71	2.44	0.47
3:B:158:LYS:O	3:B:161:ALA:N	2.48	0.47
2:F:414:DT:H5'	2:F:414:DT:C6	2.48	0.47
3:B:139:LEU:CD2	3:B:158:LYS:HB3	2.44	0.47
3:A:88:GLU:O	3:A:89:LEU:HD23	2.15	0.47
3:B:129:PRO:CG	3:B:202:ASN:HD21	2.28	0.47
1:E:315:DC:C1'	1:E:316:DA:H5''	2.45	0.46
3:B:140:ASN:HD22	3:B:143:HIS:CB	2.24	0.46
3:B:204:PHE:CD1	3:B:257:ASN:HA	2.49	0.46
2:F:417:DC:H2'	2:F:418:DC:C6	2.51	0.46
1:E:302:DT:H73	3:A:265:TYR:OH	2.15	0.46
3:B:130:GLN:OE1	3:B:141:GLN:NE2	2.43	0.46
3:B:137:THR:C	3:B:139:LEU:N	2.73	0.46
3:B:176:GLN:HB3	3:B:246:VAL:HG21	1.97	0.46
1:E:307:DT:H2''	1:E:308:DA:N7	2.30	0.46
3:A:246:VAL:HG23	3:A:247:SER:N	2.29	0.46
3:B:278:ARG:HA	3:B:278:ARG:NE	2.30	0.46
3:A:268:PHE:O	3:A:272:ARG:HG2	2.16	0.45
3:B:116:ALA:O	3:B:117:LYS:C	2.59	0.45
3:A:173:VAL:HG22	4:A:1005:HOH:O	2.16	0.45
3:A:232:LEU:HA	3:A:235:GLU:CB	2.40	0.45
1:E:316:DA:H5'	1:E:316:DA:H8	1.81	0.45
3:A:172:GLU:C	3:A:172:GLU:CD	2.84	0.45
3:A:247:SER:N	3:A:248:PRO:HD2	2.30	0.45
3:B:251:ALA:C	3:B:253:GLY:N	2.75	0.45
3:A:236:CYS:O	3:A:239:ALA:HB3	2.15	0.45
3:A:237:ASN:ND2	3:A:259:VAL:HB	2.32	0.45
3:B:233:VAL:HG23	3:B:259:VAL:HG12	1.97	0.45
2:F:402:DC:OP1	3:B:224:PRO:HB2	2.17	0.45
3:A:216:GLN:O	3:A:218:TYR:N	2.50	0.45
3:B:206:TRP:CH2	3:B:214:LEU:HD11	2.51	0.45
3:A:97:ALA:O	3:A:98:ALA:C	2.60	0.45
3:A:252:GLN:C	3:A:254:LEU:H	2.25	0.45
3:B:236:CYS:C	3:B:238:ARG:N	2.73	0.45
3:A:171:ARG:O	3:A:175:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:204:PHE:CD1	3:A:263:ARG:HD3	2.52	0.44
3:A:216:GLN:O	3:A:219:GLU:N	2.50	0.44
3:B:154:MET:HE3	3:B:158:LYS:C	2.43	0.44
3:A:107:LEU:C	3:A:109:GLN:H	2.23	0.44
3:A:228:GLU:HA	3:A:231:THR:OG1	2.17	0.44
3:B:88:GLU:C	3:B:90:GLU:H	2.26	0.44
3:B:226:LYS:HA	3:B:229:ARG:HB2	1.99	0.44
3:A:271:ARG:NH2	4:A:1071:HOH:O	2.50	0.44
3:A:225:SER:O	3:A:227:GLU:N	2.50	0.44
3:B:221:GLN:C	3:B:223:ASN:N	2.76	0.44
3:B:225:SER:C	3:B:227:GLU:H	2.26	0.44
3:B:266:ASN:N	3:B:266:ASN:HD22	2.16	0.44
2:F:414:DT:C7	3:B:146:GLN:HE22	2.31	0.44
3:A:214:LEU:O	3:A:267:TRP:CZ3	2.71	0.44
3:B:176:GLN:CG	3:B:246:VAL:HG21	2.47	0.44
2:F:402:DC:OP1	3:B:224:PRO:CG	2.66	0.44
3:B:172:GLU:C	3:B:174:ALA:N	2.72	0.44
3:B:171:ARG:C	3:B:173:VAL:N	2.74	0.44
3:B:272:ARG:C	3:B:274:GLU:H	2.26	0.44
3:B:246:VAL:O	3:B:246:VAL:CG2	2.65	0.43
3:A:229:ARG:HG2	3:A:229:ARG:NH1	2.31	0.43
3:B:95:GLU:O	3:B:98:ALA:HB3	2.18	0.43
3:A:104:VAL:HG12	3:A:108:LEU:CD1	2.48	0.43
3:B:171:ARG:O	3:B:173:VAL:N	2.51	0.43
3:A:216:GLN:C	3:A:218:TYR:N	2.76	0.43
3:A:217:ALA:O	3:A:221:GLN:C	2.61	0.43
3:A:233:VAL:HG22	3:A:261:GLU:OE2	2.19	0.43
3:B:104:VAL:O	3:B:108:LEU:HG	2.19	0.43
3:B:248:PRO:O	3:B:251:ALA:HB3	2.18	0.43
1:E:302:DT:H2''	1:E:303:DT:C5	2.53	0.43
3:A:123:LEU:HD12	3:A:128:ILE:HB	2.01	0.43
3:A:217:ALA:HB3	3:A:268:PHE:HZ	1.84	0.43
1:E:307:DT:H2''	1:E:308:DA:C8	2.54	0.43
3:A:157:GLN:O	3:A:160:ALA:HB3	2.18	0.43
3:A:214:LEU:HD13	3:A:267:TRP:CD1	2.54	0.43
3:A:168:ARG:HD3	3:A:171:ARG:HH21	1.83	0.43
3:A:201:ARG:HB2	3:A:202:ASN:H	1.61	0.43
3:B:133:VAL:HG11	3:B:144:LEU:HD21	2.01	0.43
3:B:232:LEU:O	3:B:233:VAL:C	2.62	0.43
1:E:304:DG:C2'	1:E:305:DG:C5'	2.82	0.42
1:E:301:DC:H2'	1:E:302:DT:C5	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:217:ALA:HB3	3:A:268:PHE:CZ	2.54	0.42
3:B:169:LYS:HA	3:B:171:ARG:NH1	2.35	0.42
3:B:223:ASN:ND2	3:B:225:SER:HB3	2.34	0.42
3:A:213:ILE:HD12	3:A:216:GLN:HG2	2.01	0.42
3:A:214:LEU:HD13	3:A:267:TRP:CG	2.53	0.42
3:B:104:VAL:CG2	3:B:105:GLU:N	2.82	0.42
3:B:137:THR:HB	3:B:139:LEU:HG	2.02	0.42
3:B:162:LEU:HD12	3:B:162:LEU:HA	1.79	0.42
3:B:229:ARG:C	3:B:231:THR:N	2.77	0.42
3:A:229:ARG:C	3:A:233:VAL:HG23	2.44	0.42
3:A:114:ARG:O	3:A:118:MET:HG3	2.20	0.42
3:A:132:GLU:O	3:A:136:THR:HG23	2.19	0.42
3:A:170:GLN:NE2	3:A:170:GLN:CA	2.83	0.42
3:B:142:SER:O	3:B:146:GLN:HG2	2.19	0.42
3:B:177:PHE:C	3:B:179:HIS:N	2.77	0.42
2:F:405:DG:C2'	2:F:406:DT:C5'	2.95	0.42
3:A:216:GLN:HG3	3:A:220:ARG:HH22	1.85	0.42
3:B:248:PRO:O	3:B:251:ALA:N	2.47	0.42
3:A:245:GLY:O	3:A:246:VAL:O	2.37	0.42
3:B:233:VAL:HG13	3:B:234:GLU:H	1.85	0.42
3:B:235:GLU:O	3:B:238:ARG:HB2	2.19	0.42
3:A:245:GLY:C	3:A:246:VAL:O	2.63	0.42
3:B:133:VAL:HG13	3:B:137:THR:HG21	2.02	0.42
3:B:252:GLN:NE2	4:B:1056:HOH:O	2.53	0.42
3:B:177:PHE:O	3:B:179:HIS:N	2.47	0.41
1:E:312:DA:C2'	1:E:313:DT:H5'	2.45	0.41
3:A:90:GLU:O	3:A:90:GLU:CD	2.63	0.41
3:A:170:GLN:C	3:A:172:GLU:N	2.72	0.41
3:A:213:ILE:O	3:A:216:GLN:N	2.53	0.41
3:A:221:GLN:C	3:A:223:ASN:N	2.78	0.41
3:B:125:GLN:NE2	4:B:1096:HOH:O	2.48	0.41
3:B:233:VAL:CG1	3:B:234:GLU:N	2.83	0.41
3:B:263:ARG:C	3:B:265:TYR:N	2.78	0.41
3:A:129:PRO:O	3:A:130:GLN:C	2.63	0.41
3:B:202:ASN:O	3:B:256:SER:HB2	2.20	0.41
3:B:233:VAL:HG13	3:B:234:GLU:HG3	2.03	0.41
1:E:312:DA:H1'	1:E:313:DT:C5'	2.50	0.41
2:F:401:DT:O4'	2:F:402:DC:O4'	2.38	0.41
3:A:96:GLU:O	3:A:99:HIS:HB3	2.19	0.41
3:A:112:PRO:O	3:A:116:ALA:N	2.47	0.41
2:F:402:DC:H2'	2:F:403:DT:C7	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:166:TYR:O	3:B:170:GLN:HG3	2.20	0.41
2:F:417:DC:OP1	2:F:417:DC:C4'	2.62	0.41
3:A:212:GLN:O	3:A:216:GLN:OE1	2.39	0.41
3:B:222:LYS:O	3:B:224:PRO:HD3	2.20	0.41
3:B:227:GLU:O	3:B:231:THR:OG1	2.38	0.41
3:A:224:PRO:HD3	4:A:1082:HOH:O	2.19	0.41
3:A:237:ASN:HD22	3:A:237:ASN:HA	1.63	0.41
3:B:126:HIS:HB3	4:B:1050:HOH:O	2.21	0.41
2:F:405:DG:H1'	2:F:406:DT:H5''	2.04	0.41
2:F:414:DT:H73	3:B:146:GLN:NE2	2.36	0.41
3:A:120:LYS:NZ	4:A:1004:HOH:O	2.54	0.41
3:B:163:TYR:O	3:B:166:TYR:HB3	2.21	0.41
3:B:222:LYS:O	3:B:223:ASN:C	2.64	0.41
3:A:140:ASN:HD22	3:A:143:HIS:N	2.16	0.40
3:A:140:ASN:O	3:A:143:HIS:N	2.53	0.40
3:B:223:ASN:ND2	3:B:228:GLU:OE1	2.54	0.40
3:B:252:GLN:N	3:B:252:GLN:CD	2.79	0.40
2:F:408:DA:H2''	2:F:409:DA:C5'	2.49	0.40
1:E:316:DA:C2	2:F:406:DT:N3	2.80	0.40
1:E:305:DG:H2''	1:E:306:DT:O5'	2.21	0.40
1:E:316:DA:H2	2:F:406:DT:O2	2.04	0.40
3:B:129:PRO:O	3:B:130:GLN:C	2.65	0.40
3:B:171:ARG:CG	3:B:172:GLU:H	2.29	0.40
3:B:258:LEU:HD23	3:B:258:LEU:C	2.46	0.40
3:B:263:ARG:O	3:B:264:VAL:C	2.63	0.40
1:E:319:DA:C2'	1:E:320:DG:C8	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	166/194 (86%)	126 (76%)	27 (16%)	13 (8%)	1	1
3	B	169/194 (87%)	124 (73%)	34 (20%)	11 (6%)	1	1
All	All	335/388 (86%)	250 (75%)	61 (18%)	24 (7%)	1	1

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	91	ASN
3	A	179	HIS
3	A	222	LYS
3	A	246	VAL
3	A	247	SER
3	B	246	VAL
3	B	252	GLN
3	A	245	GLY
3	A	273	LYS
3	B	89	LEU
3	B	170	GLN
3	B	172	GLU
3	B	217	ALA
3	B	222	LYS
3	A	170	GLN
3	A	226	LYS
3	A	249	SER
3	B	178	THR
3	A	216	GLN
3	B	110	GLU
3	A	110	GLU
3	A	127	ASN
3	B	247	SER
3	B	94	PRO

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	
3	A	150/169 (89%)	131 (87%)	19 (13%)	4	9
3	B	154/169 (91%)	146 (95%)	8 (5%)	21	44
All	All	304/338 (90%)	277 (91%)	27 (9%)	9	20

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	105	GLU
3	A	106	THR
3	A	109	GLN
3	A	123	LEU
3	A	124	GLN
3	A	126	HIS
3	A	142	SER
3	A	170	GLN
3	A	172	GLU
3	A	176	GLN
3	A	177	PHE
3	A	205	LYS
3	A	211	GLN
3	A	221	GLN
3	A	222	LYS
3	A	223	ASN
3	A	246	VAL
3	A	261	GLU
3	A	266	ASN
3	B	131	ARG
3	B	150	LYS
3	B	152	THR
3	B	172	GLU
3	B	177	PHE
3	B	203	ARG
3	B	227	GLU
3	B	228	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	126	HIS
3	A	127	ASN
3	A	140	ASN

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Mol	Chain	Res	Type
3	A	146	GLN
3	A	170	GLN
3	A	176	GLN
3	A	212	GLN
3	A	237	ASN
3	A	257	ASN
3	A	266	ASN
3	B	109	GLN
3	B	140	ASN
3	B	146	GLN
3	B	157	GLN
3	B	176	GLN
3	B	202	ASN
3	B	216	GLN
3	B	221	GLN
3	B	223	ASN
3	B	252	GLN
3	B	266	ASN
3	B	270	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	E	21/21 (100%)	-1.80	0 100 100	30, 46, 78, 92	0
2	F	21/21 (100%)	-1.75	0 100 100	31, 48, 78, 83	0
3	A	170/194 (87%)	-1.31	0 100 100	31, 58, 91, 96	0
3	B	173/194 (89%)	-1.31	0 100 100	28, 59, 95, 100	0
All	All	385/430 (89%)	-1.36	0 100 100	28, 59, 91, 100	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.