



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:55 AM UTC

PDB ID : 3CWT / pdb_00003cwt
Title : Crystal Structure of an AlkA Host/Guest Complex 2'-fluoro-2'-deoxyinosine:
Adenine Base Pair
Authors : Bowman, B.R.; Lee, S.; Wang, S.; Verdine, G.L.
Deposited on : 2008-04-22
Resolution : 2.30 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
Mogul : 2022.3.0, CSD as543be (2022)
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

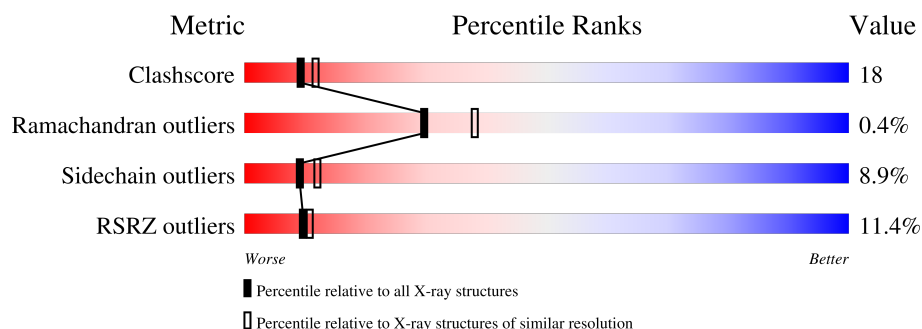
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	
1	B	282	
1	C	282	
1	D	282	
2	E	12	
2	G	12	
3	F	12	

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Mol	Chain	Length	Quality of chain
3	H	12	 67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9948 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-3-methyladenine glycosylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	B	281	Total	C	N	O	S	0	0	0
			2209	1424	386	387	12			
1	C	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	D	281	Total	C	N	O	S	0	0	0
			2209	1424	386	387	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*DGP*DAP*DCP*DAP*DTP*DGP*DAP*(2FI)P*DTP*DGP*DCP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	F	N	O	P	0	0
			245	117	1	47	69	11		
2	G	12	Total	C	F	N	O	P	0	0
			245	117	1	47	69	11		

- Molecule 3 is a DNA chain called DNA (5'-D(*DGP*DGP*DCP*DAP*DAP*DTP*DCP*DAP*DTP*DGP*DTP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			
3	H	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		

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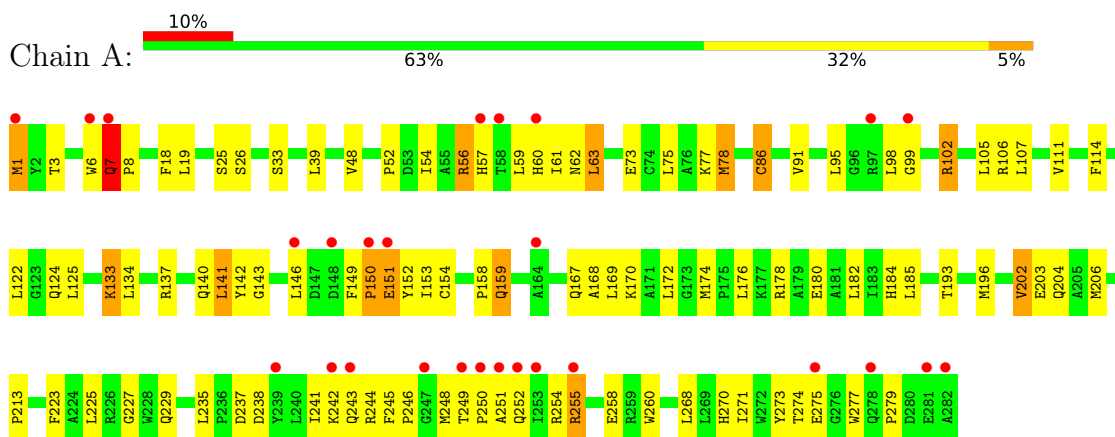
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	27	Total 27	O 27	0	0
4	C	30	Total 30	O 30	0	0
4	D	34	Total 34	O 34	0	0
4	E	1	Total 1	O 1	0	0
4	H	2	Total 2	O 2	0	0

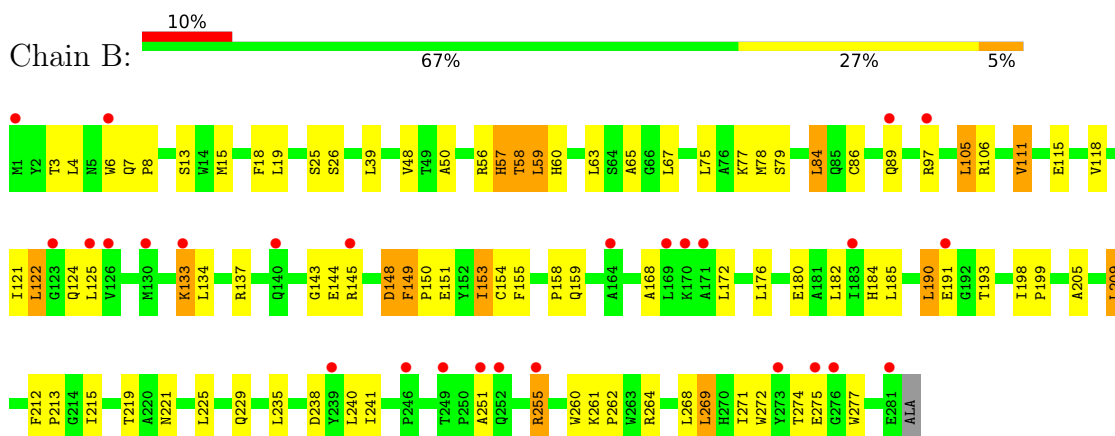
3 Residue-property plots [i](#)

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

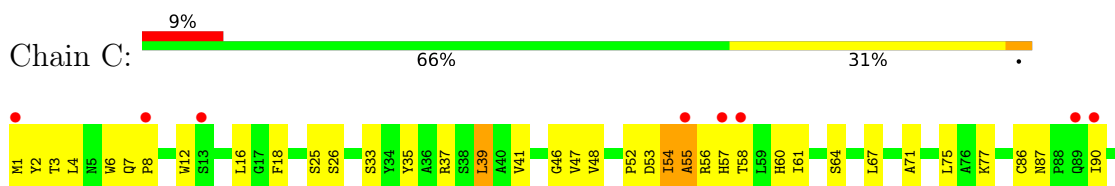
• Molecule 1: DNA-3-methyladenine glycosylase 2

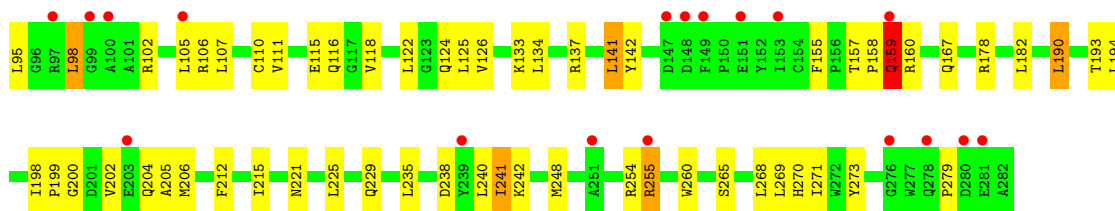


• Molecule 1: DNA-3-methyladenine glycosylase 2

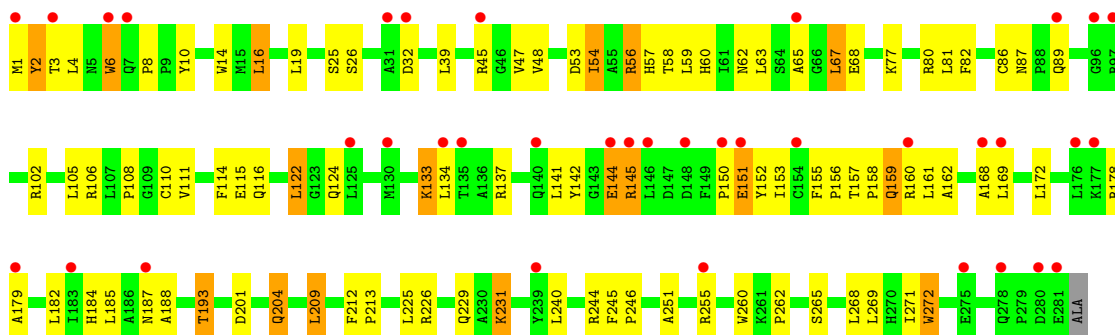


• Molecule 1: DNA-3-methyladenine glycosylase 2

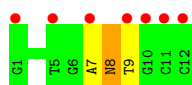
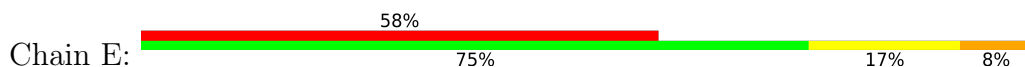




● Molecule 1: DNA-3-methyladenine glycosylase 2



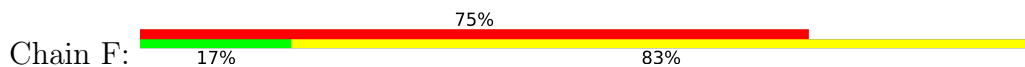
● Molecule 2: DNA (5'-D(*DGP*DAP*DCP*DAP*DTP*DGP*DAP*(2FI)P*DTP*DGP*DCP*DC)-3')



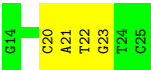
● Molecule 2: DNA (5'-D(*DGP*DAP*DCP*DAP*DTP*DGP*DAP*(2FI)P*DTP*DGP*DCP*DC)-3')



● Molecule 3: DNA (5'-D(*DGP*DGP*DCP*DAP*DAP*DTP*DCP*DAP*DTP*DGP*DTP*D C)-3')



● Molecule 3: DNA (5'-D(*DGP*DGP*DCP*DAP*DAP*DTP*DCP*DAP*DTP*DGP*DTP*D C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.75Å 101.48Å 103.11Å 90.00° 93.72° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.2 (50.00-2.30) 93.2 (50.00-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.280 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9948	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 2FI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/2277	0.99	15/3104 (0.5%)
1	B	0.48	0/2271	0.94	6/3097 (0.2%)
1	C	0.46	0/2277	0.88	5/3104 (0.2%)
1	D	0.50	0/2271	0.92	5/3097 (0.2%)
2	E	0.28	0/249	0.73	0/380
2	G	0.31	0/249	0.78	0/380
3	F	0.30	0/272	0.73	0/418
3	H	0.30	0/272	0.79	0/418
All	All	0.47	0/10138	0.91	31/13998 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	TYR	N-CA-C	-7.82	98.02	110.14
1	A	255	ARG	N-CA-C	-7.37	103.23	111.71
1	A	275	GLU	N-CA-C	7.12	119.66	111.11
1	A	7	GLN	CA-C-N	7.04	124.73	119.66
1	A	7	GLN	C-N-CA	7.04	124.73	119.66
1	B	198	ILE	N-CA-C	7.01	116.61	108.96
1	A	150	PRO	CA-C-N	-6.88	109.26	122.61
1	A	150	PRO	C-N-CA	-6.88	109.26	122.61
1	B	57	HIS	N-CA-C	-6.20	102.84	111.52
1	B	149	PHE	CA-C-N	6.17	127.55	119.84
1	B	149	PHE	C-N-CA	6.17	127.55	119.84
1	D	86	CYS	N-CA-C	6.06	119.15	110.24
1	A	152	TYR	N-CA-C	-6.04	99.05	108.90
1	B	86	CYS	N-CA-C	5.69	118.58	110.10
1	A	102	ARG	CA-C-N	5.62	125.30	119.56
1	A	102	ARG	C-N-CA	5.62	125.30	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	GLN	N-CA-C	5.54	117.32	111.28
1	C	157	THR	CA-C-N	5.50	125.33	119.28
1	C	157	THR	C-N-CA	5.50	125.33	119.28
1	A	202	VAL	N-CA-C	5.34	116.06	110.62
1	A	151	GLU	N-CA-CB	5.25	118.77	110.22
1	A	149	PHE	CA-C-N	5.16	126.29	119.84
1	A	149	PHE	C-N-CA	5.16	126.29	119.84
1	D	65	ALA	N-CA-C	5.16	116.98	111.36
1	C	86	CYS	N-CA-C	5.15	117.78	110.10
1	D	2	TYR	N-CA-C	-5.14	102.45	110.42
1	A	86	CYS	N-CA-C	5.10	117.73	110.24
1	D	245	PHE	CA-C-N	5.09	125.38	119.93
1	D	245	PHE	C-N-CA	5.09	125.38	119.93
1	A	273	TYR	N-CA-C	5.07	118.50	112.72
1	B	65	ALA	N-CA-C	5.02	117.41	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2215	0	2209	77	0
1	B	2209	0	2204	80	0
1	C	2215	0	2209	77	0
1	D	2209	0	2204	89	0
2	E	245	0	134	5	0
2	G	245	0	134	7	0
3	F	243	0	137	17	0
3	H	243	0	137	3	0
4	A	30	0	0	0	0
4	B	27	0	0	0	0
4	C	30	0	0	0	0
4	D	34	0	0	0	0
4	E	1	0	0	0	0
4	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9948	0	9368	347	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 18.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:HG22	1:A:60:HIS:HD2	1.04	1.12
1:B:133:LYS:HE3	1:B:137:ARG:HH21	1.09	1.08
1:B:143:GLY:HA3	1:B:153:ILE:HD11	1.21	1.07
1:D:54:ILE:HD12	1:D:54:ILE:H	1.19	1.05
1:B:121:ILE:HA	1:B:124:GLN:HE21	1.23	1.03
2:G:5:DT:H2''	2:G:6:DG:H5''	1.40	1.03
1:B:255:ARG:HH11	1:B:255:ARG:HB3	1.23	1.02
1:A:3:THR:HG22	1:A:60:HIS:CD2	1.97	1.00
2:E:8:2FI:H2'	2:E:9:DT:H5''	1.42	0.98
1:B:79:SER:HA	1:B:84:LEU:HD22	1.45	0.98
2:E:8:2FI:C2'	2:E:9:DT:H5''	1.96	0.94
1:B:145:ARG:HG2	1:B:145:ARG:HH11	1.35	0.91
1:B:191:GLU:OE2	1:B:193:THR:OG1	1.89	0.91
1:B:133:LYS:HE3	1:B:137:ARG:NH2	1.88	0.88
1:B:77:LYS:HB3	1:B:111:VAL:HG22	1.55	0.88
1:C:39:LEU:HD12	1:C:48:VAL:HG21	1.55	0.88
1:B:133:LYS:CE	1:B:137:ARG:HH21	1.91	0.84
1:A:3:THR:CG2	1:A:60:HIS:HD2	1.88	0.83
2:G:5:DT:H2''	2:G:6:DG:C5'	2.09	0.83
1:B:133:LYS:HD3	1:B:137:ARG:HE	1.44	0.82
1:C:107:LEU:HD11	1:C:225:LEU:HD21	1.62	0.81
1:D:54:ILE:H	1:D:54:ILE:CD1	1.92	0.81
3:F:23:DG:H2''	3:F:24:DT:H71	1.63	0.81
2:G:5:DT:C2'	2:G:6:DG:H5''	2.14	0.78
1:A:133:LYS:HD2	1:A:137:ARG:HH11	1.49	0.77
1:B:251:ALA:O	1:B:255:ARG:HG3	1.84	0.77
1:D:145:ARG:NH2	1:D:150:PRO:O	2.17	0.77
1:D:3:THR:HG22	1:D:60:HIS:HD2	1.51	0.76
1:C:124:GLN:HE21	1:C:178:ARG:HH11	1.31	0.76
2:G:4:DA:C2'	2:G:5:DT:H5''	2.15	0.75
1:D:168:ALA:O	1:D:172:LEU:HD23	1.86	0.75
1:D:188:ALA:HB1	1:D:193:THR:HG22	1.69	0.74
2:G:4:DA:H2''	2:G:5:DT:H5''	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PRO:HB2	1:B:190:LEU:HD13	1.69	0.73
2:E:8:2FI:H2'	2:E:9:DT:C5'	2.19	0.71
1:D:54:ILE:HD12	1:D:54:ILE:N	2.02	0.71
2:G:4:DA:C3'	2:G:5:DT:H5''	2.19	0.71
1:B:121:ILE:HA	1:B:124:GLN:NE2	2.02	0.70
1:B:255:ARG:HB3	1:B:255:ARG:NH1	2.03	0.70
1:C:118:VAL:O	1:C:122:LEU:HD13	1.91	0.70
1:D:108:PRO:O	1:D:226:ARG:HD2	1.91	0.70
1:C:107:LEU:HD11	1:C:225:LEU:CD2	2.20	0.70
1:D:265:SER:O	1:D:269:LEU:HD23	1.92	0.70
1:A:124:GLN:HE21	1:A:178:ARG:HH11	1.39	0.70
1:D:141:LEU:HD12	1:D:142:TYR:CE2	2.27	0.69
1:B:133:LYS:CD	1:B:137:ARG:HE	2.05	0.69
1:C:133:LYS:HE3	1:C:137:ARG:HH12	1.58	0.69
1:A:249:THR:HB	3:F:20:DC:H5'	1.74	0.68
3:F:24:DT:H2''	3:F:25:DC:H5''	1.75	0.68
3:F:24:DT:H2''	3:F:25:DC:C5'	2.23	0.68
1:D:141:LEU:HD13	1:D:141:LEU:O	1.92	0.68
1:A:6:TRP:CZ2	1:A:57:HIS:HA	2.31	0.66
1:A:91:VAL:O	1:A:95:LEU:HD23	1.95	0.66
1:A:244:ARG:C	1:A:246:PRO:HD3	2.20	0.66
1:C:53:ASP:HB3	1:C:58:THR:HG23	1.77	0.66
1:C:133:LYS:HG2	1:C:137:ARG:NH1	2.11	0.66
1:D:134:LEU:HD13	1:D:134:LEU:C	2.20	0.66
1:C:71:ALA:O	1:C:75:LEU:HD13	1.96	0.66
1:B:8:PRO:HG2	1:B:57:HIS:CE1	2.31	0.65
1:C:260:TRP:CH2	1:C:271:ILE:HD11	2.32	0.65
1:B:184:HIS:CD2	1:B:213:PRO:HD2	2.32	0.65
1:D:255:ARG:O	1:D:255:ARG:HD3	1.97	0.65
3:H:21:DA:H2''	3:H:22:DT:H5'	1.78	0.64
1:B:261:LYS:HE2	1:B:264:ARG:CZ	2.27	0.64
1:B:159:GLN:HA	1:B:190:LEU:HD21	1.80	0.64
1:A:251:ALA:HB2	3:F:20:DC:OP2	1.98	0.63
1:D:8:PRO:HG2	1:D:57:HIS:CE1	2.33	0.63
1:A:133:LYS:HD2	1:A:137:ARG:NH1	2.14	0.63
1:C:110:CYS:HB3	1:C:116:GLN:HE21	1.63	0.63
1:D:102:ARG:HG2	1:D:102:ARG:HH11	1.62	0.63
1:B:18:PHE:HD1	1:B:19:LEU:HD12	1.64	0.62
1:B:26:SER:HB3	1:B:153:ILE:HG22	1.81	0.62
1:C:158:PRO:HB2	1:C:190:LEU:HD13	1.81	0.62
1:D:77:LYS:HB3	1:D:111:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:THR:HG22	1:B:60:HIS:ND1	2.14	0.62
1:D:141:LEU:HD12	1:D:142:TYR:CD2	2.36	0.61
1:B:3:THR:C	1:B:4:LEU:HD12	2.26	0.61
1:B:122:LEU:HG	1:B:134:LEU:HD22	1.82	0.61
1:A:134:LEU:HD21	1:A:174:MET:HE2	1.82	0.61
1:A:158:PRO:HD2	1:A:159:GLN:NE2	2.16	0.61
1:A:26:SER:HB3	1:A:153:ILE:HG22	1.84	0.60
1:A:77:LYS:HB3	1:A:111:VAL:HG23	1.83	0.60
1:D:188:ALA:HB1	1:D:193:THR:CG2	2.31	0.60
1:C:212:PHE:HB3	1:C:215:ILE:HD13	1.84	0.59
1:A:122:LEU:HD13	1:A:134:LEU:HD22	1.83	0.59
1:B:261:LYS:HE2	1:B:264:ARG:NH2	2.17	0.59
1:C:133:LYS:HG2	1:C:137:ARG:HH12	1.68	0.59
1:A:1:MET:HE3	1:A:62:ASN:HB2	1.84	0.58
1:D:141:LEU:HD13	1:D:141:LEU:C	2.28	0.58
1:C:221:ASN:HB3	1:C:235:LEU:CD2	2.33	0.58
1:A:251:ALA:CB	3:F:20:DC:OP2	2.52	0.58
1:B:168:ALA:O	1:B:172:LEU:HD13	2.03	0.58
1:C:265:SER:O	1:C:269:LEU:HD23	2.03	0.58
1:C:56:ARG:HH11	1:C:56:ARG:HB3	1.68	0.58
1:B:255:ARG:HH11	1:B:255:ARG:CB	2.08	0.58
1:D:162:ALA:HB1	1:D:187:ASN:ND2	2.18	0.57
1:D:240:LEU:HD11	1:D:244:ARG:CZ	2.34	0.57
1:D:240:LEU:HD12	1:D:272:TRP:HD1	1.69	0.57
1:B:176:LEU:O	1:B:180:GLU:HG3	2.05	0.57
1:D:122:LEU:HD11	1:D:182:LEU:HD11	1.86	0.57
1:C:225:LEU:CD1	1:C:268:LEU:HD23	2.35	0.57
1:C:3:THR:C	1:C:4:LEU:HD12	2.30	0.56
1:D:157:THR:HB	1:D:159:GLN:HE21	1.70	0.56
3:F:18:DA:H1'	3:F:19:DT:H5'	1.86	0.56
3:H:22:DT:H2''	3:H:23:DG:C8	2.41	0.56
1:C:235:LEU:HG	1:C:268:LEU:HD21	1.87	0.56
3:F:18:DA:N3	3:F:18:DA:H2'	2.21	0.56
3:F:17:DA:H1'	3:F:18:DA:O5'	2.05	0.56
1:A:54:ILE:HD12	1:A:54:ILE:N	2.21	0.56
1:A:254:ARG:O	1:A:258:GLU:HG3	2.06	0.56
1:B:261:LYS:HG2	1:B:264:ARG:CZ	2.36	0.56
1:D:110:CYS:HB3	1:D:116:GLN:HE21	1.70	0.56
1:A:184:HIS:CD2	1:A:213:PRO:HD2	2.41	0.56
1:C:98:LEU:HD22	1:C:270:HIS:HB3	1.88	0.56
3:F:24:DT:H2''	3:F:25:DC:O5'	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:LEU:HD12	1:D:269:LEU:HD22	1.87	0.55
1:C:159:GLN:HG2	1:C:160:ARG:HD2	1.88	0.55
1:D:6:TRP:HZ3	1:D:58:THR:O	1.88	0.55
1:A:25:SER:O	1:A:26:SER:HB2	2.06	0.55
1:A:124:GLN:NE2	1:A:178:ARG:HH11	2.05	0.55
1:C:240:LEU:HD13	1:C:240:LEU:O	2.06	0.55
1:A:146:LEU:HD11	1:A:154:CYS:SG	2.47	0.55
1:A:140:GLN:HE21	1:A:140:GLN:HA	1.72	0.55
1:C:235:LEU:HG	1:C:268:LEU:CD2	2.37	0.55
1:C:56:ARG:HB3	1:C:56:ARG:NH1	2.22	0.55
1:B:25:SER:O	1:B:26:SER:HB2	2.07	0.54
1:D:45:ARG:NH2	1:D:144:GLU:OE2	2.41	0.54
1:A:249:THR:CB	3:F:20:DC:H5'	2.37	0.54
1:A:122:LEU:HD22	1:A:134:LEU:HD22	1.89	0.54
1:B:274:THR:CG2	1:B:277:TRP:HB2	2.38	0.54
1:C:54:ILE:O	1:C:55:ALA:C	2.50	0.54
1:C:12:TRP:O	1:C:16:LEU:HD23	2.08	0.54
1:C:47:VAL:H	1:C:64:SER:HB2	1.73	0.54
1:D:45:ARG:C	1:D:67:LEU:HD13	2.33	0.54
1:A:48:VAL:HG11	1:A:78:MET:HE3	1.90	0.53
1:C:141:LEU:HD13	1:C:142:TYR:CE2	2.42	0.53
1:C:215:ILE:HD12	1:C:215:ILE:N	2.23	0.53
1:A:169:LEU:HA	1:A:172:LEU:HD23	1.91	0.53
1:C:54:ILE:HD12	1:C:54:ILE:N	2.24	0.53
1:A:7:GLN:HG3	1:A:86:CYS:O	2.08	0.53
1:B:145:ARG:HD2	1:B:150:PRO:HA	1.90	0.53
1:C:54:ILE:H	1:C:54:ILE:CD1	2.20	0.53
1:D:14:TRP:HB2	1:D:102:ARG:HH21	1.74	0.53
1:D:25:SER:O	1:D:26:SER:HB2	2.08	0.53
1:C:255:ARG:O	1:C:255:ARG:NE	2.42	0.53
1:A:245:PHE:HB3	1:A:248:MET:HE3	1.91	0.53
1:D:260:TRP:CH2	1:D:271:ILE:HD11	2.43	0.53
1:C:212:PHE:CB	1:C:215:ILE:HD13	2.39	0.52
1:D:114:PHE:CD2	1:D:158:PRO:HG3	2.44	0.52
1:C:254:ARG:HG3	1:C:254:ARG:HH11	1.75	0.52
1:A:248:MET:HE1	1:A:279:PRO:HG3	1.91	0.52
1:B:118:VAL:HG22	1:B:182:LEU:HD22	1.91	0.52
1:B:4:LEU:HD11	1:B:75:LEU:HD22	1.91	0.52
1:B:145:ARG:HG2	1:B:145:ARG:NH1	2.11	0.52
1:C:4:LEU:HD13	1:C:61:ILE:HD12	1.91	0.52
1:D:124:GLN:NE2	1:D:178:ARG:HH11	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ILE:O	1:C:198:ILE:HG23	2.09	0.52
2:G:4:DA:H2''	2:G:5:DT:O4'	2.10	0.51
1:B:133:LYS:O	1:B:137:ARG:HG3	2.10	0.51
1:C:122:LEU:HD11	1:C:182:LEU:HD11	1.92	0.51
1:A:158:PRO:HD2	1:A:159:GLN:HE21	1.74	0.51
1:C:124:GLN:O	1:C:125:LEU:HB3	2.11	0.51
1:A:244:ARG:O	1:A:246:PRO:HD3	2.11	0.51
1:C:238:ASP:HB3	1:C:241:ILE:HB	1.91	0.51
1:B:48:VAL:HG22	1:B:63:LEU:CD2	2.41	0.51
1:C:193:THR:HG22	1:C:193:THR:O	2.10	0.51
1:B:6:TRP:CZ3	1:B:58:THR:O	2.64	0.51
1:D:240:LEU:HD11	1:D:244:ARG:NH2	2.26	0.51
1:D:53:ASP:OD2	1:D:56:ARG:HB2	2.12	0.50
1:D:39:LEU:HD22	1:D:48:VAL:HG21	1.93	0.50
1:B:6:TRP:C	1:B:6:TRP:CD1	2.89	0.50
1:C:122:LEU:CD1	1:C:182:LEU:HD21	2.42	0.50
1:A:249:THR:OG1	1:A:252:GLN:HG3	2.11	0.50
1:D:6:TRP:NE1	1:D:10:TYR:HB2	2.26	0.50
1:D:137:ARG:HB3	1:D:172:LEU:HD12	1.93	0.50
1:B:274:THR:HG22	1:B:277:TRP:HB2	1.94	0.50
1:C:54:ILE:N	1:C:54:ILE:CD1	2.75	0.50
1:D:244:ARG:C	1:D:246:PRO:HD3	2.37	0.50
1:A:6:TRP:CD1	1:A:6:TRP:C	2.90	0.49
1:D:6:TRP:CD1	1:D:6:TRP:C	2.90	0.49
2:E:8:2FI:F1'	2:E:9:DT:H5''	2.01	0.49
1:B:77:LYS:HB3	1:B:111:VAL:CG2	2.36	0.49
1:D:81:LEU:HD12	1:D:82:PHE:CE2	2.47	0.49
1:D:102:ARG:HG2	1:D:102:ARG:NH1	2.26	0.49
1:A:3:THR:CG2	1:A:60:HIS:CD2	2.76	0.49
1:B:261:LYS:HE2	1:B:264:ARG:NH1	2.27	0.49
1:C:46:GLY:HA3	1:C:67:LEU:HD22	1.95	0.49
1:D:3:THR:CG2	1:D:60:HIS:HD2	2.24	0.49
1:A:243:GLN:O	1:A:246:PRO:HG3	2.13	0.49
1:D:3:THR:HG22	1:D:60:HIS:CD2	2.41	0.49
1:C:141:LEU:HD13	1:C:142:TYR:CZ	2.48	0.49
1:D:48:VAL:HG22	1:D:63:LEU:CD1	2.43	0.49
1:B:50:ALA:HB1	1:B:59:LEU:HD21	1.95	0.49
1:D:185:LEU:HD13	1:D:185:LEU:O	2.12	0.49
1:D:105:LEU:HD23	1:D:106:ARG:N	2.28	0.48
1:D:201:ASP:CG	1:D:204:GLN:HB2	2.38	0.48
1:A:159:GLN:NE2	1:A:159:GLN:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD11	1:B:269:LEU:HB3	1.94	0.48
1:A:202:VAL:HG12	1:A:206:MET:HE2	1.94	0.48
1:D:108:PRO:O	1:D:226:ARG:CD	2.62	0.48
1:A:143:GLY:HA3	1:A:153:ILE:HD11	1.96	0.48
1:C:77:LYS:HB3	1:C:111:VAL:CG2	2.44	0.48
1:D:6:TRP:CZ3	1:D:58:THR:C	2.92	0.48
1:A:274:THR:CG2	1:A:277:TRP:HB2	2.44	0.48
1:A:122:LEU:HD22	1:A:134:LEU:CD2	2.44	0.47
1:C:225:LEU:O	1:C:229:GLN:HA	2.14	0.47
1:B:261:LYS:HG2	1:B:264:ARG:NH2	2.29	0.47
1:B:39:LEU:HD22	1:B:48:VAL:HG21	1.95	0.47
1:C:238:ASP:O	1:C:242:LYS:HG3	2.13	0.47
1:A:260:TRP:CH2	1:A:271:ILE:HD11	2.48	0.47
1:B:25:SER:O	1:B:26:SER:CB	2.62	0.47
1:A:134:LEU:HD23	1:A:134:LEU:C	2.40	0.47
1:C:6:TRP:CD1	1:C:6:TRP:C	2.92	0.47
1:B:145:ARG:HD2	1:B:150:PRO:O	2.14	0.47
1:D:6:TRP:CZ3	1:D:58:THR:O	2.67	0.47
1:C:25:SER:O	1:C:26:SER:HB2	2.15	0.47
1:C:33:SER:O	1:C:52:PRO:HD2	2.15	0.47
1:D:156:PRO:HB2	1:D:161:LEU:HD11	1.96	0.47
1:B:238:ASP:HB3	1:B:241:ILE:HB	1.96	0.46
1:D:1:MET:SD	1:D:62:ASN:HB2	2.55	0.46
1:B:8:PRO:HG2	1:B:57:HIS:ND1	2.30	0.46
1:D:255:ARG:HD3	1:D:255:ARG:C	2.40	0.46
3:F:20:DC:H2''	3:F:21:DA:H8	1.81	0.46
1:A:122:LEU:HD21	1:A:182:LEU:HD11	1.97	0.46
1:A:114:PHE:H	1:A:196:MET:HE1	1.80	0.46
1:A:168:ALA:O	1:A:172:LEU:HD22	2.15	0.46
1:B:145:ARG:NH1	1:B:145:ARG:CG	2.75	0.46
1:D:184:HIS:CD2	1:D:213:PRO:HD2	2.51	0.46
1:B:144:GLU:HB2	1:B:154:CYS:HB2	1.96	0.46
1:C:87:ASN:CG	1:C:90:ILE:HG12	2.41	0.46
1:A:255:ARG:HA	1:A:258:GLU:OE2	2.15	0.46
1:B:4:LEU:HD12	1:B:4:LEU:N	2.30	0.46
1:A:124:GLN:HE21	1:A:178:ARG:NH1	2.10	0.46
1:B:124:GLN:OE1	3:F:15:DG:H5'	2.15	0.46
1:D:122:LEU:HG	1:D:134:LEU:CD1	2.46	0.46
1:A:54:ILE:HD12	1:A:54:ILE:H	1.80	0.46
1:D:122:LEU:HG	1:D:134:LEU:HD12	1.98	0.46
1:D:134:LEU:C	1:D:134:LEU:CD1	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ALA:HB3	3:H:20:DC:OP1	2.15	0.46
1:D:151:GLU:CD	1:D:151:GLU:H	2.23	0.45
3:F:20:DC:H2''	3:F:21:DA:O5'	2.16	0.45
1:B:121:ILE:HD11	1:B:215:ILE:HG12	1.99	0.45
1:B:78:MET:CE	1:B:111:VAL:HG21	2.46	0.45
1:C:115:GLU:HG3	1:C:155:PHE:CD1	2.51	0.45
1:B:205:ALA:O	1:B:209:LEU:HD23	2.16	0.45
1:B:115:GLU:HG3	1:B:155:PHE:CE2	2.52	0.45
1:D:87:ASN:OD1	1:D:89:GLN:HB3	2.16	0.45
1:A:95:LEU:HD12	1:A:98:LEU:HD12	1.99	0.45
1:A:237:ASP:HA	1:A:242:LYS:NZ	2.32	0.45
1:B:143:GLY:HA3	1:B:153:ILE:CD1	2.16	0.45
1:D:133:LYS:HE2	1:D:133:LYS:HA	1.98	0.45
1:B:15:MET:O	1:B:19:LEU:HD13	2.16	0.45
1:C:240:LEU:HD13	1:C:240:LEU:C	2.42	0.45
1:A:223:PHE:O	1:A:227:GLY:N	2.46	0.45
1:C:241:ILE:CD1	1:C:268:LEU:HD13	2.47	0.45
1:D:63:LEU:HD22	1:D:63:LEU:N	2.32	0.45
1:D:168:ALA:O	1:D:172:LEU:CD2	2.60	0.45
1:B:190:LEU:HD12	1:C:200:GLY:HA3	1.99	0.44
1:A:33:SER:O	1:A:52:PRO:HD2	2.18	0.44
1:B:133:LYS:HD3	1:B:137:ARG:NE	2.24	0.44
1:D:6:TRP:HZ3	1:D:58:THR:C	2.25	0.44
1:D:240:LEU:HD12	1:D:272:TRP:CD1	2.50	0.44
1:A:141:LEU:HD13	1:A:142:TYR:CE2	2.52	0.44
1:A:235:LEU:HB3	1:A:238:ASP:HB2	2.00	0.44
1:C:53:ASP:HB2	1:C:60:HIS:CE1	2.52	0.44
1:D:188:ALA:CB	1:D:193:THR:HG22	2.42	0.44
1:B:56:ARG:O	1:B:57:HIS:HB2	2.18	0.44
1:B:260:TRP:CH2	1:B:271:ILE:HD11	2.53	0.44
1:C:248:MET:HE1	1:C:279:PRO:HG3	1.99	0.44
1:A:77:LYS:HD3	1:A:111:VAL:HG22	2.00	0.43
1:D:26:SER:HB3	1:D:153:ILE:HG22	2.00	0.43
1:C:77:LYS:HB3	1:C:111:VAL:HG23	2.00	0.43
1:C:199:PRO:HG3	1:C:205:ALA:CB	2.48	0.43
1:D:231:LYS:HZ2	1:D:231:LYS:HB3	1.83	0.43
1:A:18:PHE:CD1	1:A:18:PHE:C	2.96	0.43
1:A:146:LEU:HD12	1:A:146:LEU:N	2.33	0.43
1:B:115:GLU:HG3	1:B:155:PHE:CD2	2.53	0.43
1:B:121:ILE:HD13	1:B:219:THR:HG21	1.99	0.43
2:E:7:DA:H2''	2:E:8:2FI:H8	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:15:DG:H2''	3:F:16:DC:O5'	2.17	0.43
1:B:209:LEU:O	1:B:212:PHE:HB2	2.18	0.43
1:D:47:VAL:HG21	1:D:152:TYR:CD2	2.54	0.43
1:C:202:VAL:O	1:C:206:MET:HG3	2.18	0.43
1:D:115:GLU:HG3	1:D:155:PHE:CZ	2.54	0.43
1:A:61:ILE:HG22	1:A:63:LEU:HD13	2.01	0.43
1:B:199:PRO:HG3	1:B:205:ALA:CB	2.49	0.43
1:C:7:GLN:O	1:C:106:ARG:NH2	2.52	0.43
1:D:77:LYS:HB3	1:D:111:VAL:CG2	2.48	0.42
1:D:39:LEU:CD2	1:D:48:VAL:HG21	2.49	0.42
1:D:45:ARG:CZ	1:D:144:GLU:OE2	2.67	0.42
1:A:140:GLN:HA	1:A:140:GLN:NE2	2.34	0.42
1:B:6:TRP:HZ3	1:B:58:THR:O	2.01	0.42
1:B:153:ILE:HD13	1:B:154:CYS:O	2.19	0.42
1:D:141:LEU:C	1:D:141:LEU:CD1	2.92	0.42
1:A:193:THR:O	1:A:193:THR:HG22	2.20	0.42
1:B:6:TRP:CZ2	1:B:57:HIS:HA	2.54	0.42
1:C:115:GLU:HG3	1:C:155:PHE:CE1	2.55	0.42
1:D:155:PHE:CD2	1:D:156:PRO:HD2	2.54	0.42
1:A:105:LEU:HD23	1:A:105:LEU:C	2.44	0.42
1:B:225:LEU:O	1:B:229:GLN:HA	2.20	0.42
1:B:145:ARG:CD	1:B:150:PRO:O	2.67	0.42
1:B:190:LEU:HD12	1:B:190:LEU:HA	1.78	0.42
1:C:18:PHE:CD1	1:C:18:PHE:C	2.98	0.42
1:D:172:LEU:CD2	1:D:172:LEU:N	2.82	0.42
1:D:209:LEU:O	1:D:212:PHE:HB2	2.20	0.42
1:B:148:ASP:OD1	1:B:149:PHE:CD2	2.73	0.42
1:C:102:ARG:NH1	1:C:273:TYR:O	2.52	0.42
1:C:115:GLU:HG3	1:C:155:PHE:CG	2.55	0.42
1:D:2:TYR:CE2	1:D:63:LEU:HD23	2.55	0.42
3:F:18:DA:H2''	3:F:19:DT:OP2	2.20	0.42
1:C:35:TYR:OH	1:C:37:ARG:HD2	2.20	0.41
1:D:240:LEU:C	1:D:240:LEU:HD13	2.45	0.41
1:A:7:GLN:HA	1:A:8:PRO:HD3	1.83	0.41
1:A:7:GLN:CG	1:A:86:CYS:O	2.69	0.41
1:A:86:CYS:HB3	1:A:106:ARG:NE	2.35	0.41
1:C:254:ARG:HG3	1:C:254:ARG:NH1	2.35	0.41
1:D:169:LEU:HB2	1:D:179:ALA:HB1	2.01	0.41
1:D:172:LEU:N	1:D:172:LEU:HD22	2.34	0.41
1:A:73:GLU:HG2	1:D:80:ARG:NH1	2.36	0.41
1:B:159:GLN:HA	1:B:190:LEU:CD2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ARG:HG3	1:C:58:THR:HG22	2.03	0.41
1:A:167:GLN:NE2	1:A:170:LYS:HD3	2.34	0.41
1:C:105:LEU:HD11	1:C:269:LEU:HB3	2.02	0.41
1:C:255:ARG:NE	1:C:255:ARG:C	2.78	0.41
1:A:107:LEU:HD11	1:A:225:LEU:HG	2.02	0.41
1:D:124:GLN:HE21	1:D:178:ARG:HH11	1.69	0.41
1:C:56:ARG:H	1:C:56:ARG:HG2	1.72	0.41
1:D:58:THR:CG2	1:D:59:LEU:N	2.82	0.41
1:B:241:ILE:HD11	1:B:268:LEU:HD12	2.02	0.41
1:C:7:GLN:HA	1:C:8:PRO:HD3	1.94	0.41
1:A:56:ARG:C	1:A:57:HIS:CG	2.99	0.41
1:A:141:LEU:HD12	1:A:172:LEU:HD21	2.02	0.41
1:A:241:ILE:HD11	1:A:268:LEU:CD2	2.50	0.41
1:C:110:CYS:CB	1:C:116:GLN:HE21	2.33	0.41
1:C:241:ILE:HD11	1:C:268:LEU:HD13	2.02	0.41
1:A:176:LEU:HG	1:A:180:GLU:OE2	2.21	0.41
1:C:248:MET:CE	1:C:279:PRO:HG3	2.51	0.40
1:B:7:GLN:O	1:B:106:ARG:NH2	2.54	0.40
1:D:16:LEU:HD12	1:D:16:LEU:HA	1.93	0.40
1:C:41:VAL:HG22	1:C:77:LYS:HE3	2.02	0.40
1:D:25:SER:O	1:D:26:SER:CB	2.70	0.40
3:F:24:DT:C2'	3:F:25:DC:O5'	2.70	0.40
1:A:254:ARG:HH11	1:A:254:ARG:HG2	1.86	0.40
1:B:221:ASN:HB3	1:B:235:LEU:CD2	2.51	0.40
1:A:99:GLY:HA2	1:A:270:HIS:CD2	2.57	0.40
1:A:225:LEU:O	1:A:229:GLN:HA	2.22	0.40
1:D:225:LEU:O	1:D:229:GLN:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/282 (99%)	269 (96%)	11 (4%)	0	100	100
1	B	279/282 (99%)	270 (97%)	8 (3%)	1 (0%)	30	38
1	C	280/282 (99%)	266 (95%)	11 (4%)	3 (1%)	11	13
1	D	279/282 (99%)	267 (96%)	12 (4%)	0	100	100
All	All	1118/1128 (99%)	1072 (96%)	42 (4%)	4 (0%)	30	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	275	GLU
1	C	55	ALA
1	C	57	HIS
1	C	126	VAL

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	
1	A	222/222 (100%)	202 (91%)	20 (9%)	9	12
1	B	222/222 (100%)	199 (90%)	23 (10%)	7	8
1	C	222/222 (100%)	208 (94%)	14 (6%)	16	23
1	D	222/222 (100%)	200 (90%)	22 (10%)	7	9
All	All	888/888 (100%)	809 (91%)	79 (9%)	9	12

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	GLN
1	A	19	LEU
1	A	39	LEU
1	A	56	ARG
1	A	59	LEU
1	A	63	LEU

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Mol	Chain	Res	Type
1	A	75	LEU
1	A	78	MET
1	A	102	ARG
1	A	125	LEU
1	A	133	LYS
1	A	141	LEU
1	A	150	PRO
1	A	151	GLU
1	A	159	GLN
1	A	185	LEU
1	A	203	GLU
1	A	204	GLN
1	A	250	PRO
1	B	13	SER
1	B	58	THR
1	B	59	LEU
1	B	67	LEU
1	B	84	LEU
1	B	89	GLN
1	B	97	ARG
1	B	105	LEU
1	B	111	VAL
1	B	122	LEU
1	B	125	LEU
1	B	133	LYS
1	B	148	ASP
1	B	151	GLU
1	B	153	ILE
1	B	185	LEU
1	B	190	LEU
1	B	209	LEU
1	B	240	LEU
1	B	255	ARG
1	B	262	PRO
1	B	269	LEU
1	B	272	TRP
1	C	1	MET
1	C	39	LEU
1	C	54	ILE
1	C	95	LEU
1	C	98	LEU
1	C	134	LEU

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Mol	Chain	Res	Type
1	C	141	LEU
1	C	159	GLN
1	C	167	GLN
1	C	190	LEU
1	C	194	LEU
1	C	204	GLN
1	C	241	ILE
1	C	255	ARG
1	D	4	LEU
1	D	6	TRP
1	D	16	LEU
1	D	19	LEU
1	D	32	ASP
1	D	54	ILE
1	D	56	ARG
1	D	67	LEU
1	D	68	GLU
1	D	122	LEU
1	D	133	LYS
1	D	144	GLU
1	D	145	ARG
1	D	151	GLU
1	D	159	GLN
1	D	160	ARG
1	D	193	THR
1	D	204	GLN
1	D	209	LEU
1	D	231	LYS
1	D	262	PRO
1	D	272	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	85	GLN
1	A	124	GLN
1	A	140	GLN
1	A	159	GLN
1	A	167	GLN
1	A	187	ASN
1	A	204	GLN

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Mol	Chain	Res	Type
1	A	221	ASN
1	A	270	HIS
1	B	7	GLN
1	B	124	GLN
1	B	187	ASN
1	B	204	GLN
1	B	221	ASN
1	B	243	GLN
1	B	270	HIS
1	C	60	HIS
1	C	85	GLN
1	C	89	GLN
1	C	116	GLN
1	C	124	GLN
1	C	140	GLN
1	C	159	GLN
1	C	184	HIS
1	C	204	GLN
1	C	221	ASN
1	D	5	ASN
1	D	7	GLN
1	D	60	HIS
1	D	116	GLN
1	D	124	GLN
1	D	140	GLN
1	D	159	GLN
1	D	187	ASN
1	D	210	GLN
1	D	221	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	2FI	E	8	2	21,24,25	1.59	5 (23%)	30,35,38	0.85	1 (3%)
2	2FI	G	8	2	21,24,25	1.35	3 (14%)	30,35,38	1.12	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2FI	E	8	2	-	1/7/25/26	0/3/3/3
2	2FI	G	8	2	-	0/7/25/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	8	2FI	C2-N3	3.65	1.37	1.30
2	G	8	2FI	C2-N3	3.44	1.36	1.30
2	E	8	2FI	C2-N1	2.83	1.40	1.35
2	G	8	2FI	O6-C6	2.66	1.28	1.23
2	G	8	2FI	C2-N1	2.54	1.40	1.35
2	E	8	2FI	C6-N1	2.24	1.43	1.39
2	E	8	2FI	O6-C6	2.12	1.27	1.23
2	E	8	2FI	C4-N9	2.12	1.43	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	8	2FI	C2'-C1'-N9	3.63	119.85	114.27
2	G	8	2FI	O4'-C1'-C2'	-2.12	103.60	105.84
2	E	8	2FI	N1-C2-N3	-2.04	123.15	125.50

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	8	2FI	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	8	2FI	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	282/282 (100%)	0.64	27 (9%)	13 15	22, 41, 76, 101	0
1	B	281/282 (99%)	0.75	27 (9%)	13 15	26, 42, 70, 111	0
1	C	282/282 (100%)	0.71	26 (9%)	14 16	27, 44, 76, 139	0
1	D	281/282 (99%)	0.88	37 (13%)	7 8	25, 42, 67, 125	0
2	E	11/12 (91%)	2.42	7 (63%)	0 0	47, 76, 132, 142	0
2	G	11/12 (91%)	1.15	1 (9%)	15 16	47, 65, 82, 94	0
3	F	12/12 (100%)	2.50	9 (75%)	0 0	57, 119, 131, 141	0
3	H	12/12 (100%)	0.60	0	100 100	41, 57, 91, 102	0
All	All	1172/1176 (99%)	0.78	134 (11%)	10 11	22, 43, 79, 142	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	130	MET	5.7
1	D	6	TRP	5.5
2	E	9	DT	4.9
1	D	183	ILE	4.4
1	B	130	MET	4.4
1	D	140	GLN	4.3
1	C	57	HIS	4.1
1	A	282	ALA	4.0
1	C	1	MET	3.9
1	B	191	GLU	3.9
1	D	281	GLU	3.9
1	D	1	MET	3.8
1	A	1	MET	3.8
1	A	250	PRO	3.8
2	E	7	DA	3.7
1	A	151	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	6	TRP	3.6
1	B	133	LYS	3.5
3	F	19	DT	3.5
3	F	23	DG	3.4
1	C	147	ASP	3.4
1	D	187	ASN	3.4
1	A	255	ARG	3.4
1	C	153	ILE	3.3
1	C	280	ASP	3.3
3	F	24	DT	3.3
1	A	7	GLN	3.3
3	F	20	DC	3.3
1	B	171	ALA	3.2
1	C	251	ALA	3.2
1	A	148	ASP	3.2
1	A	60	HIS	3.1
1	C	58	THR	3.1
1	D	144	GLU	3.1
3	F	21	DA	3.1
1	C	90	ILE	3.1
2	E	10	DG	3.1
1	A	281	GLU	3.0
1	B	275	GLU	3.0
1	A	57	HIS	3.0
1	D	278	GLN	3.0
1	B	1	MET	3.0
1	B	246	PRO	3.0
1	B	125	LEU	3.0
1	B	169	LEU	3.0
1	C	278	GLN	3.0
1	D	7	GLN	2.9
1	B	273	TYR	2.9
2	E	11	DC	2.9
1	D	239	TYR	2.9
1	D	255	ARG	2.9
1	B	89	GLN	2.9
1	D	151	GLU	2.9
1	A	249	THR	2.9
1	A	242	LYS	2.8
1	C	97	ARG	2.8
1	D	150	PRO	2.8
1	B	255	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLY	2.8
1	C	281	GLU	2.8
1	C	203	GLU	2.8
1	B	97	ARG	2.7
1	C	55	ALA	2.7
1	D	134	LEU	2.7
1	A	243	GLN	2.7
2	E	1	DG	2.7
1	C	255	ARG	2.7
1	D	145	ARG	2.7
1	C	148	ASP	2.6
1	A	150	PRO	2.6
3	F	18	DA	2.6
2	E	12	DC	2.6
1	D	179	ALA	2.6
1	B	249	THR	2.6
1	B	239	TYR	2.6
1	B	183	ILE	2.6
1	B	140	GLN	2.6
1	C	8	PRO	2.6
1	D	146	LEU	2.5
1	A	99	GLY	2.5
1	A	278	GLN	2.5
1	D	89	GLN	2.5
1	D	168	ALA	2.5
1	C	239	TYR	2.5
3	F	22	DT	2.5
1	D	148	ASP	2.5
1	C	100	ALA	2.5
1	C	159	GLN	2.5
1	D	3	THR	2.4
3	F	14	DG	2.4
1	D	65	ALA	2.4
2	G	5	DT	2.4
1	D	280	ASP	2.4
1	A	251	ALA	2.4
1	A	58	THR	2.4
1	A	97	ARG	2.4
1	A	239	TYR	2.3
1	B	276	GLY	2.3
1	C	99	GLY	2.3
2	E	5	DT	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	45	ARG	2.3
1	A	6	TRP	2.3
1	C	89	GLN	2.3
1	C	105	LEU	2.3
1	D	154	CYS	2.3
1	B	251	ALA	2.3
1	D	32	ASP	2.2
1	A	164	ALA	2.2
1	A	247	GLY	2.2
1	D	96	GLY	2.2
1	D	275	GLU	2.2
1	D	135	THR	2.2
1	A	253	ILE	2.2
1	D	169	LEU	2.2
1	B	145	ARG	2.2
1	A	275	GLU	2.2
1	B	281	GLU	2.2
1	B	164	ALA	2.2
1	D	160	ARG	2.2
1	B	126	VAL	2.2
1	D	97	ARG	2.1
1	A	252	GLN	2.1
1	D	125	LEU	2.1
1	D	176	LEU	2.1
1	C	13	SER	2.1
1	C	149	PHE	2.1
1	B	170	LYS	2.1
1	C	151	GLU	2.1
1	C	276	GLY	2.1
1	D	31	ALA	2.0
3	F	25	DC	2.0
1	B	252	GLN	2.0
1	A	146	LEU	2.0
1	D	177	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2FI	E	8	22/23	0.87	0.27	20,20,21,22	0
2	2FI	G	8	22/23	0.93	0.20	20,20,20,22	0

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.