



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:05 PM UTC

PDB ID : 1BY4 / pdb_00001by4
Title : STRUCTURE AND MECHANISM OF THE HOMODIMERIC ASSEMBLY
OF THE RXR ON DNA
Authors : Zhao, Q.; Chasse, S.A.; Devarakonda, S.; Sierk, M.L.; Ahvazi, B.; Sigler, P.B.;
Rastinejad, F.
Deposited on : 1998-10-22
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

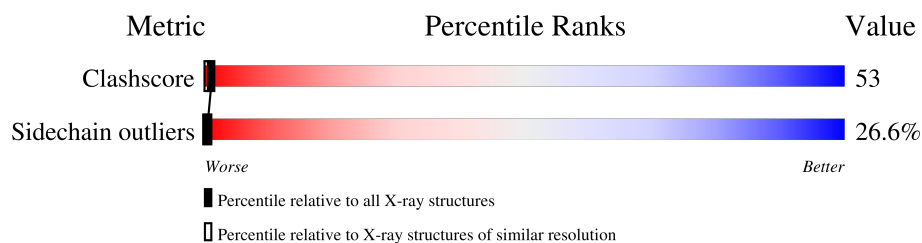
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

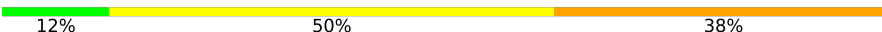
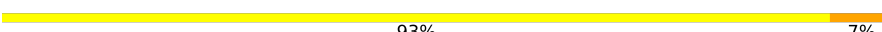
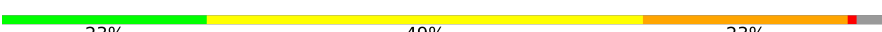
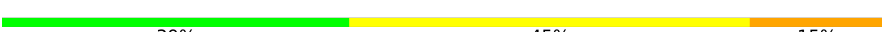
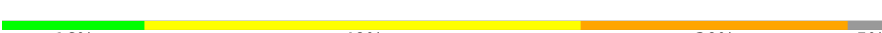
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	16	
1	G	16	
2	F	15	
2	H	15	
3	A	82	
3	B	82	
3	C	82	
3	D	82	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4062 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(*C*TP*AP*GP*GP*TP*CP*AP*AP*AP*GP*GP*TP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	15	Total	C	N	O	P	0	0	0
			310	148	62	86	14			
1	G	16	Total	C	N	O	P	0	0	0
			329	157	65	92	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			299	145	50	90	14			
2	H	15	Total	C	N	O	P	0	0	0
			299	145	50	90	14			

- Molecule 3 is a protein called PROTEIN (RETINOIC ACID RECEPTOR RXR-ALPHA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	79	Total	C	N	O	S	0	0	0
			640	387	127	115	11			
3	B	82	Total	C	N	O	S	0	0	0
			667	405	131	120	11			
3	C	78	Total	C	N	O	S	0	0	0
			629	381	123	114	11			
3	D	80	Total	C	N	O	S	0	0	0
			651	397	126	117	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1128	GLY	ALA	conflict	UNP P19793
B	1228	GLY	ALA	conflict	UNP P19793

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2128	GLY	ALA	conflict	UNP P19793
D	2228	GLY	ALA	conflict	UNP P19793

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0
4	C	2	Total Zn 2 2	0	0
4	D	2	Total Zn 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	34	Total O 34 34	0	0
5	F	43	Total O 43 43	0	0
5	G	27	Total O 27 27	0	0
5	H	39	Total O 39 39	0	0
5	A	15	Total O 15 15	0	0
5	B	32	Total O 32 32	0	0
5	C	16	Total O 16 16	0	0
5	D	24	Total O 24 24	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. 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. 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(*C*TP*AP*GP*GP*TP*CP*AP*AP*AP*GP*GP*TP*CP*AP*G)-3')

Chain E: 



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

Chain G: 

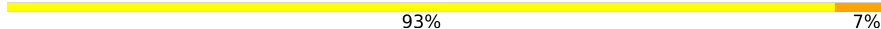


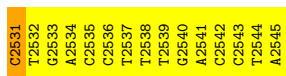
- Molecule 2: DNA (5'-D(*CP*TP*GP*AP*CP*CP*TP*TP*TP*GP*AP*CP*CP*TP*A)-3')

Chain F: 

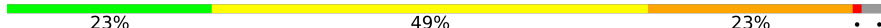


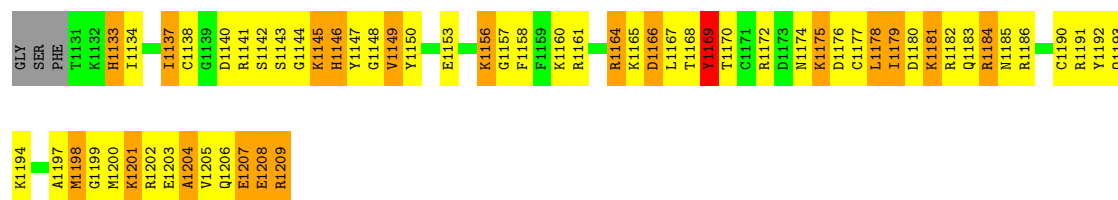
- Molecule 2: DNA (5'-D(*CP*TP*GP*AP*CP*CP*TP*TP*TP*GP*AP*CP*CP*TP*A)-3')

Chain H: 

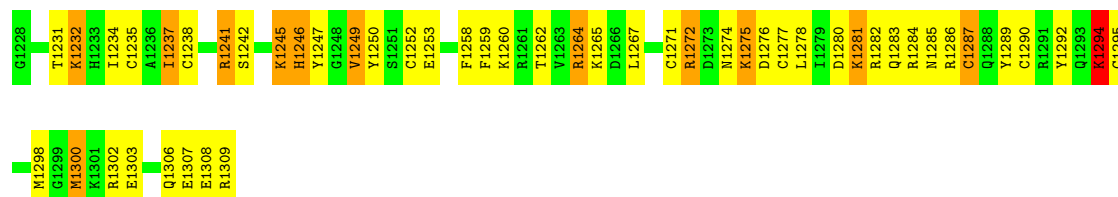


- Molecule 3: PROTEIN (RETINOIC ACID RECEPTOR RXR-ALPHA)

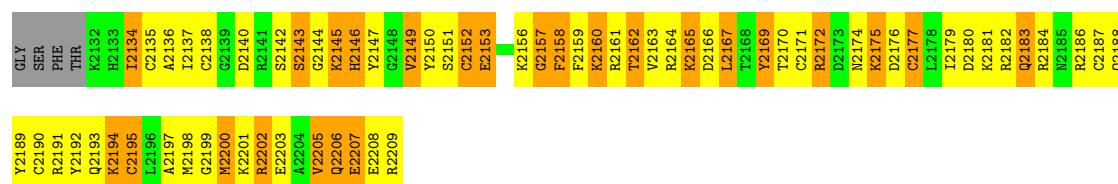
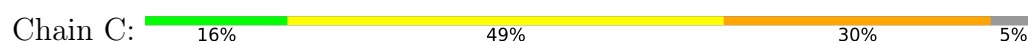
Chain A: 



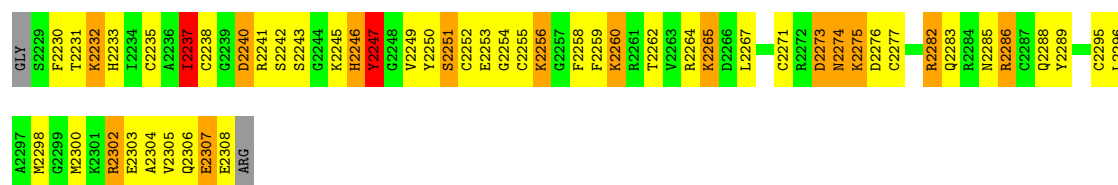
• Molecule 3: PROTEIN (RETINOIC ACID RECEPTOR RXR-ALPHA)



• Molecule 3: PROTEIN (RETINOIC ACID RECEPTOR RXR-ALPHA)



• Molecule 3: PROTEIN (RETINOIC ACID RECEPTOR RXR-ALPHA)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.93Å 33.65Å 101.40Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	72.3 (10.00-2.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.234 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4062	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.65	0/349	0.99	1/538 (0.2%)
1	G	0.72	0/370	1.19	2/570 (0.4%)
2	F	0.64	0/333	1.05	2/511 (0.4%)
2	H	0.64	0/333	0.98	1/511 (0.2%)
3	A	1.07	0/648	1.37	8/857 (0.9%)
3	B	1.05	1/676 (0.1%)	1.39	11/893 (1.2%)
3	C	1.00	1/637 (0.2%)	1.63	15/843 (1.8%)
3	D	1.05	1/660 (0.2%)	1.42	10/874 (1.1%)
All	All	0.93	3/4006 (0.1%)	1.32	50/5597 (0.9%)

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
1	E	0	2
1	G	0	4
2	F	0	4
3	C	0	1
3	D	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1249	VAL	CA-CB	5.33	1.61	1.55
3	C	2134	ILE	CA-CB	5.15	1.62	1.54
3	D	2305	VAL	CA-CB	5.10	1.61	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2207	GLU	N-CA-C	-13.23	96.58	113.12
3	C	2144	GLY	N-CA-C	-8.86	97.14	111.59
3	C	2206	GLN	N-CA-C	8.45	123.80	110.70
3	C	2197	ALA	N-CA-C	-8.18	105.29	114.62
3	A	1182	ARG	N-CA-C	8.15	119.94	111.14
3	B	1237	ILE	N-CA-C	7.98	118.87	111.45
3	C	2195	CYS	N-CA-C	-7.96	102.56	111.07
3	D	2230	PHE	N-CA-C	-7.91	103.61	113.18
3	C	2143	SER	N-CA-C	-7.48	102.73	111.03
3	C	2169	TYR	N-CA-C	7.42	120.01	108.96
3	D	2247	TYR	N-CA-C	-7.17	95.53	110.80
2	F	1531	DC	O5'-C5'-C4'	7.15	121.52	110.80
3	C	2177	CYS	N-CA-C	6.84	119.58	108.76
3	A	1169	TYR	N-CA-C	6.84	120.60	110.48
2	H	2531	DC	O5'-C5'-C4'	6.70	120.85	110.80
3	C	2200	MET	N-CA-C	-6.57	99.32	109.76
3	D	2307	GLU	N-CA-C	6.51	124.67	110.80
3	A	1185	ASN	N-CA-C	6.50	121.37	113.38
3	C	2205	VAL	N-CA-C	-6.49	106.67	112.12
3	D	2277	CYS	N-CA-C	-6.47	100.84	110.23
3	B	1277	CYS	N-CA-C	-6.34	98.28	109.06
3	A	1137	ILE	N-CA-C	6.24	120.89	113.22
3	D	2246	HIS	N-CA-C	6.18	122.41	114.56
3	B	1285	ASN	N-CA-C	6.05	120.39	113.19
3	A	1146	HIS	CA-C-N	-6.03	113.05	123.25
3	A	1146	HIS	C-N-CA	-6.03	113.05	123.25
3	B	1284	ARG	N-CA-C	5.96	117.85	111.36
3	C	2157	GLY	N-CA-C	5.87	119.77	112.73
3	B	1245	LYS	CA-C-N	-5.85	113.17	122.17
3	B	1245	LYS	C-N-CA	-5.85	113.17	122.17
1	G	2509	DG	C2'-C3'-O3'	5.74	120.11	111.50
3	D	2242	SER	N-CA-C	5.73	118.81	109.24
1	G	2494	DC	N1-C1'-C2'	5.65	121.97	113.50
3	D	2276	ASP	N-CA-C	5.51	118.34	107.98
3	B	1246	HIS	CA-C-N	-5.48	111.07	121.54
3	B	1246	HIS	C-N-CA	-5.48	111.07	121.54
3	A	1204	ALA	N-CA-C	5.47	119.95	113.28
3	B	1287	CYS	N-CA-C	5.40	116.78	109.11
3	D	2273	ASP	CB-CA-C	-5.23	108.91	116.54
1	E	1495	DT	O5'-C5'-C4'	5.20	118.61	110.80
3	C	2194	LYS	N-CA-C	-5.19	105.69	112.23
2	F	1540	DG	C5'-C4'-O4'	-5.18	101.63	109.40
3	B	1232	LYS	N-CA-C	-5.17	99.80	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1197	ALA	N-CA-C	-5.15	106.83	113.01
3	C	2152	CYS	N-CA-C	-5.12	102.61	110.14
3	D	2240	ASP	N-CA-C	-5.11	103.74	110.33
3	D	2237	ILE	N-CA-C	5.10	116.19	111.81
3	C	2146	HIS	CA-C-N	-5.09	111.82	121.54
3	C	2146	HIS	C-N-CA	-5.09	111.82	121.54
3	B	1294	LYS	N-CA-C	-5.06	105.95	111.82

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	2158	PHE	Sidechain
3	D	2247	TYR	Sidechain
1	E	1503	DA	Sidechain
1	E	1508	DA	Sidechain
2	F	1535	DC	Sidechain
2	F	1536	DC	Sidechain
2	F	1537	DT	Sidechain
2	F	1543	DC	Sidechain
1	G	2497	DG	Sidechain
1	G	2502	DA	Sidechain
1	G	2503	DA	Sidechain
1	G	2505	DG	Sidechain

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	E	310	0	170	37	0
1	G	329	0	181	31	0
2	F	299	0	172	29	0
2	H	299	0	172	33	0
3	A	640	0	619	70	0
3	B	667	0	652	61	0
3	C	629	0	606	108	0
3	D	651	0	636	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	15	0	0	2	0
5	B	32	0	0	4	0
5	C	16	0	0	2	0
5	D	24	0	0	7	0
5	E	34	0	0	4	0
5	F	43	0	0	3	0
5	G	27	0	0	1	0
5	H	39	0	0	5	0
All	All	4062	0	3208	371	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 53.

All (371) 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:H:2535:DC:H2''	2:H:2536:DC:H5''	1.13	1.09
3:C:2201:LYS:HA	3:C:2202:ARG:HH21	1.02	1.08
3:C:2202:ARG:NE	3:C:2202:ARG:H	1.54	1.04
3:C:2160:LYS:O	3:C:2164:ARG:HG2	1.57	1.04
2:F:1531:DC:H2''	2:F:1532:DT:H5'	1.38	1.01
3:D:2302:ARG:NE	3:D:2302:ARG:H	1.60	0.99
2:H:2542:DC:H2''	2:H:2543:DC:H5'	1.45	0.98
3:C:2201:LYS:HA	3:C:2202:ARG:NH2	1.80	0.94
3:C:2202:ARG:H	3:C:2202:ARG:HE	1.15	0.92
2:H:2535:DC:C2'	2:H:2536:DC:H5''	1.97	0.92
3:B:1237:ILE:HD11	3:B:1300:MET:HE1	1.50	0.91
1:G:2495:DT:H2''	1:G:2496:DA:H5''	1.49	0.91
1:E:1509:DG:H21	1:G:2494:DC:H6	1.12	0.90
3:A:1209:ARG:HB2	3:A:1209:ARG:NH1	1.88	0.89
3:B:1241:ARG:HB2	5:B:3141:HOH:O	1.70	0.89
3:D:2302:ARG:H	3:D:2302:ARG:HE	1.23	0.87
3:A:1201:LYS:H	3:A:1201:LYS:HD2	1.39	0.86
3:A:1201:LYS:HD2	3:A:1201:LYS:N	1.90	0.85
3:B:1249:VAL:HG11	3:B:1300:MET:HE2	1.61	0.83
3:B:1272:ARG:HG2	3:C:2207:GLU:CD	2.04	0.83
2:F:1531:DC:H2''	2:F:1532:DT:C5'	2.07	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1496:DA:H2''	1:E:1497:DG:H5'	1.61	0.81
3:D:2235:CYS:SG	3:D:2237:ILE:HG12	2.21	0.81
3:C:2143:SER:HB2	3:C:2146:HIS:NE2	1.96	0.81
3:B:1272:ARG:HB3	3:C:2208:GLU:CD	2.05	0.81
2:F:1541:DA:H2''	2:F:1542:DC:C5'	2.11	0.81
3:B:1272:ARG:HG2	3:C:2207:GLU:OE2	1.81	0.80
3:D:2238:CYS:SG	3:D:2240:ASP:HB2	2.23	0.79
3:C:2159:PHE:HE2	3:C:2205:VAL:HG21	1.47	0.79
2:F:1541:DA:H2''	2:F:1542:DC:H5'	1.63	0.79
3:A:1167:LEU:HD23	3:A:1169:TYR:CE2	2.18	0.79
3:C:2201:LYS:HG3	3:C:2202:ARG:NH2	1.98	0.78
3:D:2282:ARG:HA	3:D:2282:ARG:HH11	1.48	0.78
3:C:2164:ARG:NH2	3:C:2209:ARG:O	2.18	0.76
3:C:2184:ARG:HD2	3:C:2191:ARG:NH2	2.02	0.75
1:E:1503:DA:H2''	5:E:3188:HOH:O	1.86	0.75
3:B:1271:CYS:HB2	3:B:1289:TYR:CD2	2.22	0.74
2:H:2537:DT:H2''	2:H:2538:DT:H5'	1.67	0.74
3:B:1249:VAL:CG1	3:B:1300:MET:HE2	2.17	0.74
3:C:2158:PHE:CD1	3:C:2191:ARG:HD3	2.23	0.74
3:B:1237:ILE:O	3:B:1294:LYS:NZ	2.20	0.73
3:A:1138:CYS:SG	3:A:1184:ARG:NH1	2.62	0.72
3:D:2271:CYS:HB2	3:D:2289:TYR:CD2	2.25	0.72
3:D:2247:TYR:HB2	3:D:2300:MET:HE2	1.70	0.72
1:G:2496:DA:H2'	1:G:2497:DG:C8	2.25	0.72
3:D:2302:ARG:HE	3:D:2302:ARG:N	1.87	0.72
1:E:1503:DA:H2''	1:E:1504:DG:OP2	1.87	0.72
3:B:1280:ASP:HA	5:B:3355:HOH:O	1.89	0.72
3:A:1179:ILE:HD11	3:A:1190:CYS:HB3	1.71	0.71
3:C:2201:LYS:CA	3:C:2202:ARG:HH21	1.92	0.71
3:A:1147:TYR:O	3:A:1200:MET:HA	1.91	0.71
3:A:1209:ARG:HB2	3:A:1209:ARG:CZ	2.19	0.71
3:C:2157:GLY:O	3:C:2161:ARG:HB2	1.91	0.71
3:B:1272:ARG:HB2	3:C:2207:GLU:O	1.91	0.71
1:E:1496:DA:C2'	1:E:1497:DG:H5'	2.20	0.70
3:B:1275:LYS:O	3:B:1290:CYS:SG	2.49	0.70
3:C:2201:LYS:HG3	3:C:2202:ARG:HH22	1.55	0.70
3:B:1265:LYS:HB2	3:B:1267:LEU:HG	1.74	0.70
3:D:2246:HIS:HB2	3:D:2251:SER:OG	1.92	0.69
3:B:1262:THR:HG23	3:B:1267:LEU:HB2	1.75	0.69
3:A:1164:ARG:NH1	3:A:1165:LYS:HE3	2.07	0.69
3:A:1181:LYS:C	3:A:1181:LYS:HE3	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1264:ARG:HG2	3:B:1264:ARG:HH11	1.57	0.69
3:D:2235:CYS:HB2	3:D:2252:CYS:H	1.57	0.68
1:E:1508:DA:H2''	1:E:1509:DG:C5'	2.24	0.68
3:C:2199:GLY:HA2	5:C:3149:HOH:O	1.93	0.67
1:G:2499:DT:H4'	1:G:2500:DC:OP1	1.94	0.67
3:A:1184:ARG:HD2	3:A:1191:ARG:NH2	2.08	0.67
3:C:2138:CYS:SG	3:C:2140:ASP:HB2	2.34	0.67
3:D:2235:CYS:HB2	3:D:2252:CYS:N	2.10	0.67
3:B:1264:ARG:HG2	3:B:1264:ARG:NH1	2.10	0.66
3:C:2177:CYS:SG	3:C:2187:CYS:CB	2.83	0.66
3:C:2183:GLN:HA	3:D:2308:GLU:OE1	1.95	0.66
3:B:1271:CYS:SG	3:B:1274:ASN:O	2.53	0.66
3:A:1207:GLU:O	3:A:1209:ARG:HG2	1.95	0.66
3:C:2189:TYR:CD2	3:C:2190:CYS:N	2.63	0.66
2:H:2542:DC:H5''	5:H:3123:HOH:O	1.94	0.66
1:E:1495:DT:H5'	3:A:1146:HIS:CE1	2.32	0.65
3:C:2137:ILE:HD11	3:C:2198:MET:HB2	1.79	0.65
2:H:2541:DA:C8	3:C:2153:GLU:HG3	2.32	0.65
3:D:2304:ALA:HA	5:D:3293:HOH:O	1.96	0.65
3:C:2159:PHE:CE2	3:C:2205:VAL:HG21	2.30	0.65
3:A:1153:GLU:OE1	3:A:1156:LYS:HD3	1.97	0.64
3:D:2283:GLN:O	3:D:2286:ARG:HB2	1.96	0.64
3:A:1158:PHE:CG	3:A:1191:ARG:HD3	2.32	0.64
3:B:1292:TYR:HA	3:B:1295:CYS:HB2	1.79	0.64
3:D:2285:ASN:HA	5:D:3129:HOH:O	1.97	0.64
3:C:2146:HIS:CG	3:C:2156:LYS:HD3	2.34	0.63
3:B:1286:ARG:NH1	3:C:2207:GLU:HB2	2.13	0.63
1:E:1503:DA:H61	2:F:1537:DT:H3	1.47	0.63
3:A:1181:LYS:O	3:A:1184:ARG:HG3	1.98	0.63
3:B:1280:ASP:HB2	5:B:3273:HOH:O	1.99	0.63
3:C:2177:CYS:SG	3:C:2187:CYS:HB2	2.39	0.62
1:E:1495:DT:C6	1:E:1495:DT:H5''	2.34	0.62
3:B:1264:ARG:HH11	3:B:1264:ARG:CG	2.11	0.62
3:C:2170:THR:HG23	3:C:2170:THR:O	1.98	0.62
1:G:2496:DA:N6	2:H:2543:DC:C4	2.67	0.62
3:B:1272:ARG:CB	3:C:2208:GLU:HB2	2.29	0.62
3:A:1183:GLN:HE22	3:A:1186:ARG:NH2	1.98	0.62
1:G:2496:DA:H5'	3:C:2156:LYS:HZ3	1.64	0.62
3:C:2135:CYS:N	3:C:2140:ASP:O	2.30	0.62
1:E:1507:DC:H1'	1:E:1508:DA:N7	2.15	0.61
1:G:2504:DG:H2''	1:G:2505:DG:H5'	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1190:CYS:O	3:A:1194:LYS:HB2	2.00	0.61
3:B:1286:ARG:NH1	3:C:2207:GLU:CB	2.64	0.61
3:B:1295:CYS:O	3:B:1300:MET:HB2	2.01	0.61
2:F:1540:DG:N7	3:A:1161:ARG:NH2	2.48	0.61
1:G:2503:DA:OP2	3:D:2246:HIS:O	2.18	0.61
3:C:2202:ARG:HE	3:C:2202:ARG:N	1.93	0.61
3:C:2135:CYS:HB3	3:C:2140:ASP:H	1.64	0.61
3:A:1158:PHE:HE1	3:A:1192:TYR:HB2	1.66	0.60
3:B:1237:ILE:HG23	3:B:1294:LYS:HG2	1.83	0.60
2:F:1541:DA:H1'	2:F:1542:DC:H5''	1.83	0.60
1:G:2496:DA:C2'	1:G:2497:DG:C8	2.84	0.60
1:E:1508:DA:H2''	1:E:1509:DG:H5'	1.82	0.60
3:C:2203:GLU:HA	3:C:2206:GLN:HB2	1.84	0.60
2:H:2544:DT:H2''	2:H:2545:DA:OP2	2.02	0.60
2:F:1543:DC:H6	2:F:1543:DC:H5'	1.67	0.59
2:F:1541:DA:C2'	2:F:1542:DC:H5''	2.33	0.59
3:A:1153:GLU:OE1	3:A:1156:LYS:CD	2.50	0.59
2:H:2534:DA:H2''	5:H:3177:HOH:O	2.03	0.59
3:D:2274:ASN:N	3:D:2274:ASN:OD1	2.34	0.59
3:A:1186:ARG:HH21	3:B:1308:GLU:CD	2.11	0.59
3:B:1264:ARG:C	3:B:1265:LYS:HD3	2.27	0.58
1:G:2496:DA:OP2	3:C:2146:HIS:O	2.21	0.58
1:G:2498:DG:H2''	1:G:2499:DT:H5'	1.84	0.58
2:H:2540:DG:N7	3:C:2161:ARG:NH2	2.52	0.58
3:B:1307:GLU:O	3:B:1309:ARG:NH1	2.36	0.58
3:A:1156:LYS:HG2	3:A:1157:GLY:N	2.19	0.58
2:F:1543:DC:H5'	2:F:1543:DC:C6	2.39	0.58
1:E:1503:DA:OP2	3:B:1246:HIS:O	2.22	0.58
1:G:2496:DA:H5'	3:C:2156:LYS:NZ	2.18	0.58
1:G:2503:DA:H2''	1:G:2504:DG:OP2	2.04	0.58
2:F:1541:DA:H2''	2:F:1542:DC:H5''	1.86	0.57
3:C:2158:PHE:CG	3:C:2191:ARG:HD3	2.39	0.57
3:C:2186:ARG:HB2	3:D:2308:GLU:OE2	2.04	0.57
3:A:1145:LYS:NZ	3:A:1148:GLY:H	2.03	0.57
3:C:2160:LYS:C	3:C:2164:ARG:HG2	2.29	0.57
3:C:2186:ARG:HB3	5:C:3184:HOH:O	2.03	0.57
3:B:1237:ILE:CD1	3:B:1300:MET:HE1	2.29	0.57
3:D:2237:ILE:HG21	3:D:2295:CYS:HA	1.87	0.56
3:D:2247:TYR:OH	3:D:2260:LYS:HG3	2.04	0.56
3:C:2137:ILE:HD12	3:C:2195:CYS:HA	1.86	0.56
3:A:1166:ASP:OD1	3:A:1166:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1199:GLY:O	3:A:1201:LYS:HG3	2.05	0.56
1:G:2508:DA:H2''	1:G:2509:DG:C5'	2.36	0.56
2:H:2539:DT:H2''	2:H:2540:DG:C8	2.41	0.56
1:G:2497:DG:H2''	1:G:2498:DG:OP2	2.06	0.56
2:F:1544:DT:H2'	5:F:3007:HOH:O	2.07	0.55
2:F:1537:DT:H1'	2:F:1538:DT:H5''	1.88	0.55
3:D:2237:ILE:HG13	3:D:2255:CYS:SG	2.47	0.55
1:E:1509:DG:N2	1:G:2494:DC:C6	2.65	0.55
3:B:1265:LYS:HD3	3:B:1265:LYS:N	2.22	0.55
3:C:2137:ILE:CD1	3:C:2198:MET:HB2	2.35	0.55
3:C:2203:GLU:C	3:C:2205:VAL:H	2.14	0.55
2:H:2541:DA:N7	3:C:2153:GLU:HG3	2.22	0.55
3:C:2202:ARG:O	3:C:2205:VAL:HB	2.06	0.55
1:G:2496:DA:H4'	1:G:2496:DA:OP1	2.05	0.55
3:D:2302:ARG:H	3:D:2302:ARG:CD	2.19	0.55
3:B:1271:CYS:HB2	3:B:1289:TYR:HD2	1.72	0.54
3:C:2159:PHE:HE2	3:C:2205:VAL:CG2	2.19	0.54
2:F:1535:DC:N4	3:B:1253:GLU:OE1	2.33	0.54
3:B:1286:ARG:HH11	3:C:2207:GLU:H	1.54	0.54
1:G:2495:DT:C2'	1:G:2496:DA:H5''	2.31	0.54
3:C:2137:ILE:CD1	3:C:2195:CYS:HA	2.37	0.54
3:A:1186:ARG:HE	3:B:1308:GLU:CD	2.15	0.54
3:C:2192:TYR:O	3:C:2195:CYS:HB2	2.07	0.54
2:H:2531:DC:H2'	2:H:2532:DT:H71	1.90	0.54
5:E:3314:HOH:O	3:A:1209:ARG:HG3	2.06	0.53
3:A:1165:LYS:O	3:A:1167:LEU:HD12	2.08	0.53
3:B:1286:ARG:NH1	3:C:2207:GLU:H	2.06	0.53
3:C:2138:CYS:SG	3:C:2140:ASP:CB	2.96	0.53
3:C:2138:CYS:SG	3:C:2184:ARG:NH1	2.82	0.53
3:C:2159:PHE:O	3:C:2163:VAL:HG23	2.08	0.53
3:D:2295:CYS:O	3:D:2300:MET:HG3	2.09	0.53
3:A:1145:LYS:HG2	3:A:1146:HIS:N	2.24	0.53
1:E:1495:DT:H2'	1:E:1496:DA:N7	2.25	0.52
1:G:2508:DA:H2''	1:G:2509:DG:H5'	1.92	0.52
1:E:1495:DT:H2'	1:E:1496:DA:C8	2.44	0.52
3:C:2137:ILE:HD12	3:C:2194:LYS:O	2.08	0.52
3:D:2238:CYS:SG	3:D:2240:ASP:CB	2.97	0.52
1:E:1503:DA:H4'	3:B:1306:GLN:NE2	2.25	0.52
3:C:2149:VAL:CG1	3:C:2200:MET:HG2	2.40	0.52
3:D:2265:LYS:NZ	3:D:2267:LEU:HD11	2.25	0.52
3:A:1209:ARG:HB2	3:A:1209:ARG:HH11	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2186:ARG:NH2	3:D:2308:GLU:HB3	2.24	0.51
3:A:1191:ARG:HG2	3:A:1191:ARG:O	2.10	0.51
3:C:2171:CYS:HB3	3:C:2174:ASN:C	2.36	0.51
2:H:2535:DC:H2''	2:H:2536:DC:H6	1.76	0.51
3:A:1176:ASP:O	3:A:1177:CYS:C	2.53	0.51
3:B:1247:TYR:HB2	3:B:1300:MET:HG3	1.91	0.51
3:A:1158:PHE:CE1	3:A:1192:TYR:HB2	2.45	0.51
3:C:2171:CYS:HB3	3:C:2174:ASN:O	2.11	0.51
3:A:1137:ILE:HD12	3:A:1137:ILE:H	1.75	0.51
3:C:2147:TYR:OH	3:C:2160:LYS:HE3	2.10	0.51
3:C:2175:LYS:HD2	3:C:2189:TYR:CE2	2.46	0.51
3:D:2302:ARG:NE	3:D:2302:ARG:N	2.42	0.51
1:G:2496:DA:H2'	1:G:2497:DG:N7	2.26	0.51
3:B:1272:ARG:HB3	3:C:2208:GLU:HB2	1.91	0.51
3:B:1272:ARG:HB3	3:C:2208:GLU:OE1	2.10	0.51
3:B:1286:ARG:HH11	3:C:2207:GLU:N	2.09	0.51
3:D:2233:HIS:HD2	5:D:3287:HOH:O	1.93	0.51
3:B:1280:ASP:OD1	3:B:1283:GLN:HG2	2.11	0.50
3:A:1137:ILE:HG22	3:A:1137:ILE:O	2.11	0.50
3:B:1286:ARG:HH11	3:C:2207:GLU:HB2	1.77	0.50
3:A:1179:ILE:HD11	3:A:1190:CYS:CB	2.38	0.50
3:C:2201:LYS:O	3:C:2205:VAL:HG23	2.12	0.50
2:F:1532:DT:H2''	2:F:1533:DG:C8	2.47	0.49
1:E:1509:DG:H5'	1:E:1509:DG:H8	1.78	0.49
2:H:2542:DC:C4	2:H:2543:DC:N4	2.81	0.49
3:C:2142:SER:HA	3:C:2151:SER:O	2.11	0.49
3:A:1164:ARG:CZ	3:A:1165:LYS:HE3	2.43	0.49
3:C:2165:LYS:O	3:C:2167:LEU:N	2.45	0.49
3:D:2245:LYS:NZ	5:D:3196:HOH:O	2.44	0.49
1:E:1496:DA:OP2	3:A:1146:HIS:O	2.31	0.49
1:G:2495:DT:H2''	1:G:2496:DA:C5'	2.33	0.49
3:D:2271:CYS:HB2	3:D:2289:TYR:HD2	1.77	0.49
3:A:1164:ARG:O	3:A:1166:ASP:N	2.37	0.49
3:B:1258:PHE:CE1	3:B:1292:TYR:HB2	2.48	0.49
3:B:1259:PHE:CD2	3:B:1300:MET:HG2	2.48	0.49
3:B:1272:ARG:CG	3:C:2207:GLU:CD	2.80	0.49
3:C:2170:THR:O	3:C:2171:CYS:C	2.56	0.49
3:A:1165:LYS:O	3:A:1166:ASP:C	2.55	0.48
3:A:1193:GLN:NE2	5:A:3171:HOH:O	2.34	0.48
3:A:1199:GLY:O	3:A:1200:MET:C	2.55	0.48
2:H:2537:DT:H2''	2:H:2538:DT:C5'	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1165:LYS:O	3:A:1167:LEU:CD1	2.61	0.48
3:A:1192:TYR:C	3:A:1192:TYR:CD2	2.92	0.48
3:C:2136:ALA:HB3	3:C:2149:VAL:CG2	2.43	0.48
3:C:2175:LYS:HD2	3:C:2189:TYR:OH	2.13	0.48
3:D:2246:HIS:CD2	3:D:2256:LYS:HD2	2.48	0.48
3:B:1281:LYS:HE2	3:B:1281:LYS:O	2.14	0.48
3:D:2245:LYS:HA	3:D:2250:TYR:HA	1.95	0.48
3:D:2262:THR:HA	3:D:2267:LEU:HD12	1.96	0.48
1:G:2496:DA:C2	1:G:2497:DG:C2	3.02	0.48
1:E:1509:DG:N2	1:G:2494:DC:C5	2.82	0.47
3:B:1235:CYS:HB2	3:B:1252:CYS:N	2.28	0.47
3:A:1207:GLU:O	3:A:1209:ARG:CG	2.61	0.47
3:B:1238:CYS:O	3:B:1280:ASP:HA	2.15	0.47
3:C:2146:HIS:ND1	3:C:2156:LYS:HD3	2.29	0.47
3:C:2189:TYR:HD2	3:C:2190:CYS:SG	2.37	0.47
2:F:1534:DA:C2	2:F:1535:DC:C2	3.03	0.47
1:G:2505:DG:H2'	5:G:3127:HOH:O	2.15	0.47
2:H:2535:DC:H2''	2:H:2536:DC:C6	2.49	0.47
3:C:2158:PHE:O	3:C:2162:THR:OG1	2.32	0.47
1:G:2502:DA:H2''	1:G:2503:DA:H8	1.80	0.47
3:C:2177:CYS:SG	3:C:2187:CYS:HB3	2.50	0.47
3:C:2202:ARG:O	3:C:2206:GLN:N	2.47	0.47
2:F:1536:DC:H2''	2:F:1537:DT:OP2	2.16	0.46
2:H:2536:DC:H4'	2:H:2536:DC:OP1	2.16	0.46
3:A:1178:LEU:N	3:A:1178:LEU:HD23	2.29	0.46
3:A:1184:ARG:CD	3:A:1191:ARG:NH2	2.78	0.46
3:D:2232:LYS:HB2	3:D:2233:HIS:H	1.46	0.46
3:C:2177:CYS:HB2	3:C:2190:CYS:SG	2.55	0.46
2:H:2535:DC:H2''	2:H:2536:DC:C5'	2.09	0.46
3:B:1259:PHE:CE2	3:B:1300:MET:HG2	2.50	0.46
3:C:2152:CYS:O	3:C:2156:LYS:HB3	2.15	0.46
3:A:1201:LYS:N	3:A:1201:LYS:CD	2.62	0.46
3:A:1180:ASP:O	3:A:1181:LYS:C	2.59	0.45
3:C:2175:LYS:HB3	3:C:2175:LYS:HE3	1.32	0.45
3:D:2265:LYS:HZ2	3:D:2267:LEU:HD11	1.81	0.45
3:C:2147:TYR:CD1	3:C:2205:VAL:HG22	2.51	0.45
3:A:1149:VAL:HG13	3:A:1200:MET:HG2	1.97	0.45
1:E:1496:DA:C2	2:F:1545:DA:C2	3.04	0.45
3:A:1167:LEU:HD23	3:A:1169:TYR:HE2	1.72	0.45
3:D:2231:THR:O	5:D:3263:HOH:O	2.20	0.45
3:D:2243:SER:HB2	5:D:3042:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1496:DA:H1'	1:E:1497:DG:H5'	1.99	0.45
3:C:2180:ASP:O	3:C:2184:ARG:HB3	2.16	0.45
3:C:2189:TYR:HD2	3:C:2190:CYS:N	2.11	0.45
1:E:1508:DA:H2''	1:E:1509:DG:H5''	1.99	0.45
3:A:1167:LEU:HD23	3:A:1169:TYR:CZ	2.52	0.45
3:A:1183:GLN:NE2	3:A:1186:ARG:NH2	2.65	0.45
3:C:2163:VAL:HG11	3:C:2206:GLN:HG3	1.99	0.45
1:E:1498:DG:H2'	1:E:1499:DT:C7	2.47	0.45
3:C:2202:ARG:O	3:C:2206:GLN:HB2	2.16	0.45
3:D:2259:PHE:HE1	3:D:2296:LEU:HD23	1.81	0.45
1:E:1507:DC:H1'	1:E:1508:DA:C5	2.52	0.45
3:A:1156:LYS:HZ3	3:A:1156:LYS:HG3	1.51	0.45
2:F:1532:DT:H4'	1:G:2494:DC:C4	2.51	0.44
3:C:2203:GLU:C	3:C:2205:VAL:N	2.75	0.44
3:D:2235:CYS:SG	3:D:2237:ILE:CG1	2.99	0.44
3:D:2264:ARG:NE	3:D:2306:GLN:O	2.50	0.44
3:A:1174:ASN:O	3:A:1175:LYS:C	2.58	0.44
3:D:2258:PHE:HE2	3:D:2288:GLN:NE2	2.15	0.44
1:E:1507:DC:O3'	1:E:1508:DA:C8	2.70	0.44
1:E:1500:DC:H1'	1:E:1501:DA:N7	2.32	0.44
3:A:1138:CYS:SG	3:A:1140:ASP:HB2	2.56	0.44
3:D:2282:ARG:HD2	3:D:2282:ARG:N	2.32	0.44
2:H:2536:DC:H2'	2:H:2537:DT:H71	1.99	0.44
3:A:1147:TYR:HD1	3:A:1204:ALA:HB1	1.83	0.44
1:E:1503:DA:N6	2:F:1537:DT:H3	2.15	0.44
3:A:1137:ILE:HD12	3:A:1137:ILE:N	2.33	0.44
3:B:1245:LYS:HG2	3:B:1250:TYR:CD1	2.52	0.44
3:C:2165:LYS:O	3:C:2166:ASP:C	2.59	0.44
3:C:2170:THR:O	3:C:2170:THR:CG2	2.63	0.44
3:D:2296:LEU:HA	5:D:3337:HOH:O	2.18	0.44
3:A:1206:GLN:NE2	5:A:3279:HOH:O	2.51	0.44
2:H:2537:DT:H2'	2:H:2538:DT:H72	1.99	0.44
3:C:2179:ILE:HG23	3:C:2184:ARG:HA	2.00	0.44
1:E:1507:DC:H1'	1:E:1508:DA:C8	2.53	0.43
3:B:1286:ARG:HG3	3:C:2207:GLU:HB2	2.00	0.43
3:C:2158:PHE:HA	3:C:2161:ARG:NH1	2.33	0.43
1:E:1502:DA:H2''	5:E:3034:HOH:O	2.18	0.43
2:F:1545:DA:H1'	5:F:3359:HOH:O	2.17	0.43
2:F:1542:DC:H2''	2:F:1543:DC:H5'	2.00	0.43
2:H:2533:DG:H2'	3:D:2254:GLY:HA2	2.00	0.43
3:B:1276:ASP:O	3:B:1276:ASP:OD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2137:ILE:HD12	3:C:2194:LYS:C	2.44	0.43
2:H:2534:DA:H2''	2:H:2535:DC:H5''	1.99	0.43
3:A:1164:ARG:HD3	3:A:1165:LYS:HG3	1.99	0.43
3:B:1307:GLU:O	3:B:1308:GLU:O	2.37	0.43
2:F:1544:DT:H6	5:F:3007:HOH:O	2.00	0.43
2:H:2534:DA:C2'	5:H:3177:HOH:O	2.63	0.43
2:H:2537:DT:H1'	2:H:2538:DT:H5''	2.00	0.43
3:A:1133:HIS:ND1	3:A:1150:TYR:CE1	2.87	0.43
3:A:1140:ASP:OD2	3:A:1141:ARG:N	2.49	0.43
3:A:1142:SER:OG	3:A:1144:GLY:O	2.37	0.43
2:H:2538:DT:C2'	2:H:2539:DT:H71	2.48	0.43
3:C:2169:TYR:CE1	3:C:2188:GLN:NE2	2.87	0.42
1:E:1496:DA:C1'	1:E:1497:DG:H5'	2.49	0.42
1:E:1500:DC:H1'	1:E:1501:DA:C8	2.53	0.42
1:G:2501:DA:C2	2:H:2540:DG:N2	2.86	0.42
2:F:1541:DA:C2'	2:F:1542:DC:C5'	2.86	0.42
2:H:2539:DT:H2''	2:H:2540:DG:H8	1.84	0.42
2:F:1536:DC:H2''	2:F:1537:DT:H72	2.00	0.42
1:G:2502:DA:H2''	1:G:2503:DA:C8	2.55	0.42
3:A:1174:ASN:O	3:A:1176:ASP:N	2.53	0.42
3:C:2146:HIS:HD2	3:C:2151:SER:HB2	1.84	0.42
3:B:1295:CYS:O	3:B:1300:MET:HE3	2.20	0.42
3:A:1158:PHE:CD2	3:A:1191:ARG:HD3	2.53	0.42
3:B:1287:CYS:O	3:B:1289:TYR:N	2.52	0.42
3:C:2137:ILE:O	3:C:2137:ILE:HG22	2.19	0.42
3:D:2259:PHE:HE1	3:D:2296:LEU:CD2	2.33	0.42
2:F:1542:DC:H2''	2:F:1543:DC:C6	2.55	0.42
3:C:2186:ARG:HH21	3:D:2308:GLU:HB3	1.84	0.42
2:F:1531:DC:C2'	2:F:1532:DT:H5'	2.29	0.41
1:G:2505:DG:OP2	3:D:2264:ARG:NH2	2.44	0.41
3:B:1260:LYS:O	3:B:1264:ARG:HB2	2.19	0.41
3:C:2151:SER:OG	3:C:2200:MET:CE	2.68	0.41
1:G:2496:DA:P	3:C:2146:HIS:O	2.78	0.41
2:H:2542:DC:C2'	2:H:2543:DC:H5'	2.32	0.41
3:B:1245:LYS:HG2	3:B:1250:TYR:CE1	2.55	0.41
3:B:1247:TYR:HB2	3:B:1300:MET:CG	2.49	0.41
2:F:1541:DA:C1'	2:F:1542:DC:H5''	2.47	0.41
3:C:2179:ILE:HD12	3:C:2179:ILE:H	1.85	0.41
3:A:1137:ILE:HG13	3:A:1198:MET:HG2	2.02	0.41
1:E:1503:DA:C2'	5:E:3188:HOH:O	2.58	0.41
2:H:2536:DC:H5	5:H:3178:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1208:GLU:H	3:A:1208:GLU:HG3	1.38	0.41
3:C:2201:LYS:CG	3:C:2202:ARG:NH2	2.78	0.41
1:E:1497:DG:N2	2:F:1544:DT:C2	2.88	0.41
1:E:1502:DA:H2'	5:B:3120:HOH:O	2.20	0.41
2:H:2531:DC:H2''	2:H:2532:DT:C6	2.56	0.41
3:A:1149:VAL:HG23	3:A:1150:TYR:N	2.36	0.41
3:B:1234:ILE:HD13	3:B:1234:ILE:HA	1.95	0.41
3:D:2237:ILE:HG12	3:D:2237:ILE:H	1.68	0.41
1:E:1503:DA:P	3:B:1246:HIS:O	2.79	0.41
1:G:2494:DC:H2''	1:G:2495:DT:O5'	2.19	0.41
3:C:2164:ARG:NE	3:C:2164:ARG:HA	2.36	0.41
2:H:2538:DT:H2''	2:H:2539:DT:OP2	2.20	0.40
3:C:2172:ARG:HH11	3:C:2172:ARG:HG2	1.86	0.40
3:A:1179:ILE:H	3:A:1179:ILE:HG12	1.72	0.40
3:D:2273:ASP:HB3	3:D:2274:ASN:H	1.59	0.40
2:H:2531:DC:H5''	5:H:3074:HOH:O	2.21	0.40
1:E:1495:DT:C6	1:E:1495:DT:C5'	3.01	0.40
1:E:1498:DG:C8	1:E:1499:DT:H72	2.57	0.40
3:C:2145:LYS:HA	3:C:2150:TYR:HA	2.03	0.40
3:C:2189:TYR:CD2	3:C:2189:TYR:C	2.97	0.40
3:C:2199:GLY:O	3:C:2201:LYS:HD2	2.22	0.40
3:D:2274:ASN:HB2	3:D:2275:LYS:H	1.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	68/72 (94%)	42 (62%)	26 (38%)	0	0
3	B	72/72 (100%)	57 (79%)	15 (21%)	1	0
3	C	67/72 (93%)	51 (76%)	16 (24%)	1	0
3	D	71/72 (99%)	54 (76%)	17 (24%)	1	0
All	All	278/288 (96%)	204 (73%)	74 (27%)	0	0

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1133	HIS
3	A	1134	ILE
3	A	1143	SER
3	A	1145	LYS
3	A	1149	VAL
3	A	1156	LYS
3	A	1160	LYS
3	A	1164	ARG
3	A	1166	ASP
3	A	1168	THR
3	A	1169	TYR
3	A	1170	THR
3	A	1172	ARG
3	A	1175	LYS
3	A	1178	LEU
3	A	1179	ILE
3	A	1181	LYS
3	A	1184	ARG
3	A	1198	MET
3	A	1201	LYS
3	A	1202	ARG
3	A	1203	GLU
3	A	1205	VAL
3	A	1207	GLU
3	A	1208	GLU
3	A	1209	ARG
3	B	1231	THR
3	B	1232	LYS
3	B	1241	ARG
3	B	1242	SER
3	B	1264	ARG
3	B	1272	ARG
3	B	1275	LYS

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Mol	Chain	Res	Type
3	B	1278	LEU
3	B	1281	LYS
3	B	1282	ARG
3	B	1294	LYS
3	B	1298	MET
3	B	1300	MET
3	B	1302	ARG
3	B	1303	GLU
3	C	2134	ILE
3	C	2145	LYS
3	C	2149	VAL
3	C	2153	GLU
3	C	2160	LYS
3	C	2162	THR
3	C	2165	LYS
3	C	2167	LEU
3	C	2172	ARG
3	C	2175	LYS
3	C	2176	ASP
3	C	2181	LYS
3	C	2182	ARG
3	C	2183	GLN
3	C	2193	GLN
3	C	2202	ARG
3	D	2232	LYS
3	D	2237	ILE
3	D	2241	ARG
3	D	2249	VAL
3	D	2251	SER
3	D	2253	GLU
3	D	2256	LYS
3	D	2260	LYS
3	D	2265	LYS
3	D	2274	ASN
3	D	2275	LYS
3	D	2282	ARG
3	D	2286	ARG
3	D	2298	MET
3	D	2302	ARG
3	D	2303	GLU
3	D	2307	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	1183	GLN
3	B	1246	HIS
3	B	1306	GLN
3	C	2183	GLN
3	C	2188	GLN
3	D	2233	HIS
3	D	2246	HIS
3	D	2283	GLN
3	D	2288	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.