



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:23 AM UTC

PDB ID : 5FDK / pdb_00005fdk
Title : Crystal structure of RecU(D88N) in complex with palindromic DNA duplex
Authors : Khavnekar, S.; Rafferty, J.B.; Kale, A.
Deposited on : 2015-12-16
Resolution : 3.21 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

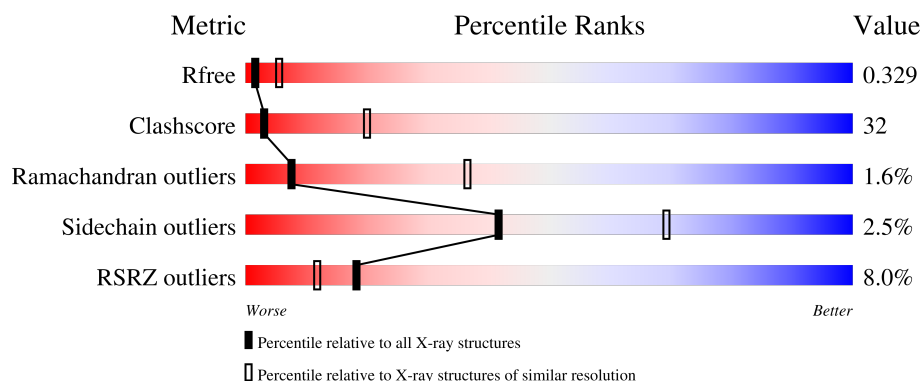
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	199	11% 47% 34% 8% 11%
1	B	199	6% 49% 29% 17%
1	C	199	4% 46% 37% 13%
1	D	199	9% 58% 36% 6%
2	E	12	17% 83%

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Mol	Chain	Length	Quality of chain
2	F	12	17%67%17%
2	G	12	8%50%33%8%8%
2	H	12	8%33%50%8%8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6138 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 Holliday junction resolvase RecU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1313	845	216	250	2			
1	B	166	Total	C	N	O	S	0	0	0
			1238	793	200	244	1			
1	C	174	Total	C	N	O	S	0	0	0
			1278	815	214	247	2			
1	D	199	Total	C	N	O	S	0	0	0
			1366	863	229	272	2			

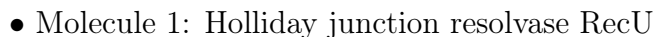
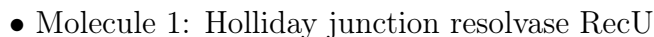
There are 4 discrepancies between the modelled and reference sequences:

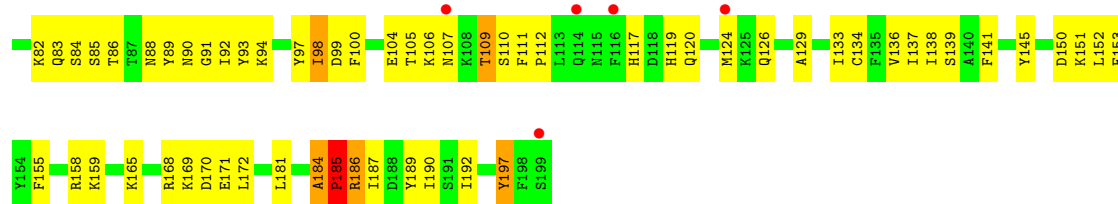
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	ASN	ASP	engineered mutation	UNP P39792
B	88	ASN	ASP	engineered mutation	UNP P39792
C	88	ASN	ASP	engineered mutation	UNP P39792
D	88	ASN	ASP	engineered mutation	UNP P39792

- Molecule 2 is a DNA chain called palindromic DNA.

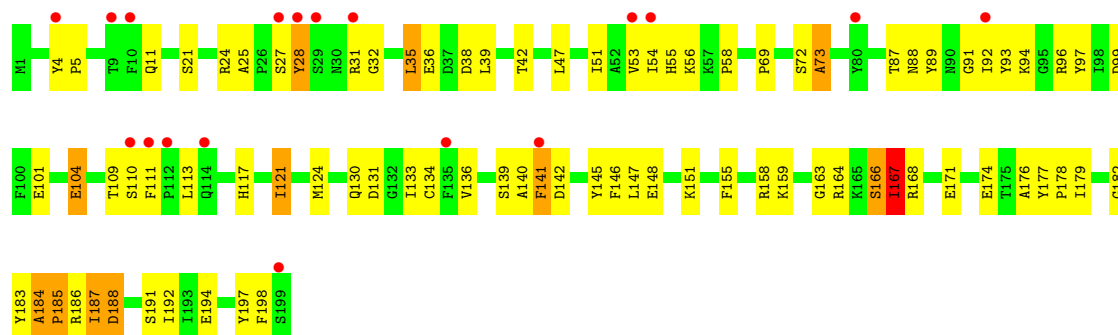
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	P	0	0	0
			246	117	45	72	12			
2	F	12	Total	C	N	O	P	0	0	0
			246	117	45	72	12			
2	G	11	Total	C	N	O	P	0	0	0
			225	107	40	67	11			
2	H	11	Total	C	N	O	P	0	0	0
			226	107	43	65	11			

- Molecule 1: Holliday junction resolvase RecU

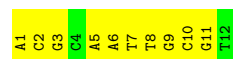




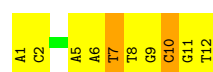
● Molecule 1: Holliday junction resolvase RecU



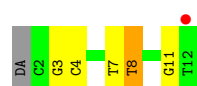
● Molecule 2: palindromic DNA



● Molecule 2: palindromic DNA



● Molecule 2: palindromic DNA



● Molecule 2: palindromic DNA



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	144.45Å 144.45Å 310.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.69 – 3.21 48.69 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.69-3.21) 99.7 (48.69-3.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.256 , 0.329 0.272 , 0.329	Depositor DCC
R_{free} test set	1063 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	119.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 113.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6138	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.42% 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	A	0.91	1/1347 (0.1%)	1.49	25/1840 (1.4%)
1	B	0.90	1/1265 (0.1%)	1.74	23/1728 (1.3%)
1	C	0.79	0/1311	1.25	13/1794 (0.7%)
1	D	0.82	3/1398 (0.2%)	1.37	23/1923 (1.2%)
2	E	0.43	0/275	1.25	2/422 (0.5%)
2	F	0.38	0/275	1.29	3/422 (0.7%)
2	G	0.29	0/251	1.08	1/385 (0.3%)
2	H	0.29	0/253	1.15	3/388 (0.8%)
All	All	0.80	5/6375 (0.1%)	1.42	93/8902 (1.0%)

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	A	0	2
1	B	0	2
1	D	0	2
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	SER	C-N	10.01	1.47	1.33
1	D	167	ILE	C-N	8.83	1.47	1.33
1	D	5	PRO	N-CD	-8.65	1.35	1.47
1	A	47	LEU	CA-C	6.31	1.61	1.52
1	B	185	PRO	N-CD	5.58	1.55	1.47

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	SER	CA-C-N	-21.29	78.69	121.91
1	B	72	SER	C-N-CA	-21.29	78.69	121.91
1	B	72	SER	CB-CA-C	20.60	145.04	110.43
1	B	72	SER	N-CA-C	-18.14	80.48	108.42
1	A	38	ASP	N-CA-C	14.19	126.25	111.07
1	A	186	ARG	N-CA-C	-13.99	81.00	110.80
1	B	167	ILE	N-CA-C	12.97	126.56	107.37
1	B	64	VAL	N-CA-C	12.03	121.12	111.62
1	D	104	GLU	N-CA-C	12.01	128.58	107.80
1	D	187	ILE	N-CA-C	-11.92	84.54	109.34
1	A	47	LEU	N-CA-C	11.80	135.93	110.80
1	C	41	GLU	N-CA-C	-11.17	99.47	113.55
1	D	188	ASP	N-CA-CB	11.09	128.69	111.39
1	A	46	TYR	N-CA-C	-10.43	99.99	111.36
1	D	142	ASP	N-CA-C	10.36	125.72	111.74
1	A	158	ARG	N-CA-C	-9.84	100.51	111.14
1	A	37	ASP	CA-C-N	-9.80	107.70	120.44
1	A	37	ASP	C-N-CA	-9.80	107.70	120.44
1	D	188	ASP	N-CA-C	-9.32	98.72	111.87
1	B	71	ARG	N-CA-C	9.30	121.19	111.14
1	C	43	ASN	N-CA-C	9.20	121.31	111.28
1	A	91	GLY	N-CA-C	9.09	122.27	110.45
1	C	187	ILE	N-CA-C	-8.66	91.33	109.34
2	H	6	DA	OP2-P-O3'	-8.59	82.25	108.00
1	D	141	PHE	N-CA-C	8.53	128.97	110.80
2	H	6	DA	OP1-P-O3'	-8.26	83.22	108.00
1	A	48	THR	N-CA-C	8.07	128.00	110.80
1	A	36	GLU	N-CA-C	-7.78	103.24	112.89
1	A	186	ARG	CB-CA-C	7.78	125.90	110.42
1	A	118	ASP	N-CA-C	7.63	119.23	111.07
1	B	197	TYR	N-CA-C	7.42	121.60	112.54
1	D	21	SER	N-CA-C	7.16	120.81	109.50
1	B	114	GLN	N-CA-C	-7.12	104.72	113.19
1	D	104	GLU	N-CA-CB	-7.01	99.97	110.90
2	E	8	DT	N1-C1'-C2'	6.95	123.93	113.50
1	B	88	ASN	N-CA-C	6.80	118.69	111.28
1	C	137	ILE	N-CA-C	6.71	117.29	107.37
1	B	74	ALA	N-CA-C	6.65	124.97	110.80
1	C	35	LEU	CA-C-O	6.63	125.63	119.00
1	B	64	VAL	CB-CA-C	-6.60	105.17	111.05
1	D	72	SER	N-CA-C	-6.59	97.03	108.69
1	D	142	ASP	N-CA-CB	-6.56	102.22	112.13
1	C	66	VAL	CB-CA-C	-6.55	104.62	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	185	PRO	N-CA-C	-6.50	99.08	112.47
1	D	140	ALA	N-CA-C	6.43	120.38	110.42
1	A	48	THR	N-CA-CB	-6.41	99.66	110.49
1	D	167	ILE	CA-C-N	-6.22	111.76	123.27
1	D	167	ILE	C-N-CA	-6.22	111.76	123.27
1	B	151	LYS	N-CA-C	-6.20	104.15	111.03
1	B	104	GLU	N-CA-C	6.15	119.27	108.75
1	C	185	PRO	CA-N-CD	-6.06	103.52	112.00
2	F	10	DC	C3'-C2'-C1'	-6.05	92.52	101.60
1	C	186	ARG	N-CA-C	5.99	117.81	111.28
1	A	64	VAL	N-CA-C	5.98	116.16	110.42
1	D	166	SER	O-C-N	5.97	129.74	122.88
1	B	175	THR	N-CA-C	5.96	118.54	111.33
1	B	172	LEU	N-CA-C	-5.96	104.71	111.14
1	A	184	ALA	CA-C-N	-5.92	112.44	119.84
1	A	184	ALA	C-N-CA	-5.92	112.44	119.84
1	B	166	SER	N-CA-C	5.79	117.76	109.14
1	B	75	VAL	N-CA-C	5.70	116.93	109.58
1	D	104	GLU	CB-CA-C	-5.70	102.31	110.62
1	B	168	ARG	N-CA-CB	5.69	118.34	109.97
1	C	82	LYS	N-CA-C	-5.65	100.83	109.65
2	G	8	DT	C1'-O4'-C4'	-5.63	101.25	109.70
2	F	10	DC	C2'-C3'-O3'	-5.62	103.07	111.50
1	A	118	ASP	CB-CA-C	-5.56	102.15	110.88
1	A	135	PHE	N-CA-C	5.55	115.57	108.24
1	C	100	PHE	N-CA-C	5.53	115.14	107.73
1	D	4	TYR	CA-C-N	-5.51	112.96	119.84
1	D	4	TYR	C-N-CA	-5.51	112.96	119.84
1	C	184	ALA	O-C-N	5.44	124.68	120.38
1	A	142	ASP	N-CA-C	-5.38	103.81	111.24
1	A	192	ILE	N-CA-C	-5.32	106.50	111.45
1	D	187	ILE	CB-CA-C	5.31	120.00	111.29
1	B	69	PRO	CA-N-CD	-5.29	104.60	112.00
1	A	116	PHE	N-CA-C	-5.27	102.95	110.59
1	C	88	ASN	N-CA-C	5.25	119.86	112.72
2	F	7	DT	P-O5'-C5'	-5.23	112.16	120.00
1	C	109	THR	CB-CA-C	-5.23	100.02	110.42
1	A	65	ASN	N-CA-C	5.21	116.92	108.26
1	A	130	GLN	N-CA-C	-5.21	103.27	110.35
1	B	162	ASN	N-CA-C	5.20	118.37	111.30
1	D	27	SER	N-CA-C	5.16	121.78	110.80
1	A	187	ILE	CB-CA-C	-5.15	105.06	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	DA	O4'-C1'-N9	5.11	116.06	108.40
2	E	9	DG	O4'-C1'-C2'	-5.11	98.74	106.40
1	B	37	ASP	N-CA-C	-5.10	105.17	111.40
1	B	185	PRO	CA-N-CD	-5.08	104.89	112.00
1	D	168	ARG	N-CA-CB	-5.08	102.88	110.60
1	A	43	ASN	N-CA-C	5.06	116.79	111.28
1	D	35	LEU	N-CA-C	-5.04	107.19	113.55
1	D	73	ALA	N-CA-C	5.03	116.16	108.52

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	TYR	Peptide
1	A	33	MET	Peptide
1	B	184	ALA	Peptide
1	B	72	SER	Peptide
1	D	11	GLN	Peptide
1	D	184	ALA	Peptide

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	1313	0	1119	98	0
1	B	1238	0	1081	66	0
1	C	1278	0	1046	65	0
1	D	1366	0	1030	100	1
2	E	246	0	136	9	0
2	F	246	0	136	14	0
2	G	225	0	125	3	1
2	H	226	0	124	5	0
All	All	6138	0	4797	342	1

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 32.

All (342) 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:B:69:PRO:CG	1:B:73:ALA:HA	1.43	1.44
1:B:69:PRO:CD	1:B:74:ALA:H	1.30	1.41
1:B:69:PRO:HG2	1:B:73:ALA:CA	1.62	1.29
1:B:69:PRO:HG2	1:B:72:SER:O	1.38	1.23
1:D:69:PRO:HB2	1:D:73:ALA:CB	1.76	1.16
1:B:69:PRO:HD3	1:B:74:ALA:N	1.66	1.11
1:D:69:PRO:CD	1:D:73:ALA:HB1	1.81	1.11
1:B:69:PRO:CD	1:B:74:ALA:N	2.12	1.11
1:D:69:PRO:HD2	1:D:73:ALA:HB1	1.20	1.09
1:D:69:PRO:HB2	1:D:73:ALA:HB2	1.13	1.08
1:A:36:GLU:O	1:A:40:ASN:CB	2.01	1.06
1:A:39:LEU:O	1:A:43:ASN:ND2	1.89	1.05
1:D:69:PRO:CB	1:D:73:ALA:CB	2.38	1.01
1:B:69:PRO:HD3	1:B:74:ALA:H	0.85	1.01
1:A:36:GLU:O	1:A:40:ASN:HB3	1.61	0.99
1:A:135:PHE:CD2	1:A:146:PHE:CE1	2.51	0.99
1:B:69:PRO:CG	1:B:72:SER:O	2.08	0.97
1:B:69:PRO:CG	1:B:73:ALA:CA	2.32	0.95
1:D:69:PRO:HD2	1:D:73:ALA:CB	1.98	0.94
1:D:166:SER:O	1:D:167:ILE:HG13	1.68	0.93
1:D:69:PRO:CD	1:D:73:ALA:CB	2.47	0.92
1:D:124:MET:HE3	1:D:134:CYS:SG	2.11	0.91
1:A:36:GLU:O	1:A:40:ASN:HB2	1.72	0.89
1:A:184:ALA:CB	1:A:185:PRO:HD2	2.02	0.88
1:A:184:ALA:HB3	1:A:185:PRO:HD2	1.57	0.85
1:C:159:LYS:HG3	1:C:165:LYS:HA	1.57	0.85
1:A:40:ASN:HA	1:A:43:ASN:HD22	1.41	0.85
1:A:86:THR:HG23	1:A:123:HIS:CE1	2.12	0.84
1:D:69:PRO:O	1:D:73:ALA:HB3	1.77	0.84
1:A:184:ALA:CB	1:A:185:PRO:CD	2.55	0.84
1:B:69:PRO:HD2	1:B:74:ALA:H	1.39	0.83
1:A:135:PHE:CE2	1:A:146:PHE:HE1	1.97	0.82
1:D:184:ALA:HB1	1:D:186:ARG:HB2	1.61	0.82
1:D:183:TYR:HA	1:D:184:ALA:HB2	1.60	0.81
1:A:184:ALA:HB1	1:A:185:PRO:CD	2.11	0.81
1:A:33:MET:CB	1:A:34:THR:HA	2.12	0.80
1:A:34:THR:N	1:A:38:ASP:HB2	1.97	0.80
1:A:33:MET:N	1:A:34:THR:OG1	2.14	0.79
1:D:69:PRO:CG	1:D:73:ALA:HB1	2.13	0.78
1:A:34:THR:H	1:A:38:ASP:HB2	1.48	0.78
2:F:6:DA:H1'	2:F:7:DT:H5''	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:HIS:CD2	1:A:127:VAL:CG2	2.68	0.77
1:C:34:THR:HG22	1:C:36:GLU:H	1.50	0.77
1:A:185:PRO:O	1:A:187:ILE:N	2.17	0.76
1:D:124:MET:CE	1:D:134:CYS:SG	2.73	0.76
1:D:104:GLU:OE1	1:D:104:GLU:O	2.04	0.76
1:A:135:PHE:CE2	1:A:146:PHE:CE1	2.73	0.76
1:A:90:ASN:HD21	1:C:90:ASN:HD21	1.33	0.76
1:A:135:PHE:CD2	1:A:146:PHE:HE1	2.02	0.76
1:D:184:ALA:CB	1:D:186:ARG:HB2	2.16	0.76
1:D:24:ARG:CB	1:D:25:ALA:HB2	2.17	0.75
1:A:185:PRO:O	1:A:186:ARG:C	2.27	0.73
1:B:69:PRO:HG2	1:B:72:SER:C	2.13	0.73
1:C:184:ALA:HB3	1:C:185:PRO:HD3	1.69	0.73
1:A:123:HIS:CD2	1:A:127:VAL:HG21	2.24	0.73
1:C:60:PRO:HG2	1:C:84:SER:HB3	1.70	0.73
1:A:157:ASP:O	1:A:161:LYS:CG	2.37	0.72
1:A:40:ASN:HA	1:A:43:ASN:ND2	2.05	0.72
1:C:136:VAL:HG21	1:C:152:LEU:HD22	1.72	0.71
1:D:69:PRO:CG	1:D:73:ALA:CB	2.69	0.71
1:D:186:ARG:O	1:D:186:ARG:HG2	1.90	0.70
1:D:179:ILE:HA	1:D:192:ILE:HD11	1.74	0.70
1:D:54:ILE:HA	1:D:91:GLY:HA3	1.74	0.69
1:D:111:PHE:N	1:D:167:ILE:O	2.18	0.69
1:B:83:GLN:O	1:B:85:SER:N	2.24	0.69
1:A:32:GLY:C	1:A:104:GLU:OE1	2.36	0.69
1:B:86:THR:HG21	1:D:55:HIS:CD2	2.27	0.69
1:D:69:PRO:N	1:D:73:ALA:HB3	2.08	0.69
1:D:69:PRO:CB	1:D:73:ALA:HB2	2.02	0.68
2:F:8:DT:H1'	2:F:9:DG:H5'	1.73	0.68
1:D:35:LEU:HD22	1:D:139:SER:CB	2.23	0.67
1:A:56:LYS:HB2	1:A:89:TYR:CE2	2.29	0.67
1:A:90:ASN:ND2	1:C:90:ASN:HD21	1.91	0.67
1:B:38:ASP:O	1:B:42:THR:OG1	2.10	0.67
2:E:3:DG:H1	2:F:10:DC:H42	1.42	0.67
1:B:66:VAL:HG13	1:B:76:ILE:HG13	1.77	0.67
1:C:53:VAL:HB	1:C:92:ILE:HG22	1.76	0.67
1:B:86:THR:HG21	1:D:55:HIS:HD2	1.61	0.66
1:C:93:TYR:CE1	1:C:94:LYS:HG2	2.29	0.66
1:C:110:SER:HB2	1:C:168:ARG:HA	1.77	0.66
1:A:118:ASP:OD1	1:A:118:ASP:N	2.29	0.66
1:D:183:TYR:CA	1:D:184:ALA:HB2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:HIS:CD2	1:A:127:VAL:HG23	2.32	0.65
1:D:183:TYR:HA	1:D:184:ALA:CB	2.23	0.65
1:A:164:ARG:NH2	2:F:6:DA:OP1	2.30	0.65
1:D:69:PRO:CA	1:D:73:ALA:HB3	2.27	0.65
1:D:155:PHE:CD2	1:D:167:ILE:HD13	2.32	0.65
1:B:69:PRO:HD2	1:B:74:ALA:N	2.00	0.64
1:C:93:TYR:CD1	1:C:94:LYS:HG2	2.33	0.64
1:A:40:ASN:CA	1:A:43:ASN:HD22	2.11	0.64
1:B:101:GLU:HB3	1:B:136:VAL:HA	1.80	0.63
1:A:184:ALA:HB1	1:A:185:PRO:HD2	1.78	0.63
1:A:183:TYR:O	1:A:184:ALA:HB3	1.97	0.63
1:D:166:SER:C	1:D:167:ILE:HG13	2.24	0.62
1:C:109:THR:OG1	1:C:110:SER:N	2.23	0.62
1:B:42:THR:HG22	1:B:46:TYR:CE2	2.34	0.62
1:A:33:MET:CB	1:A:35:LEU:HD12	2.30	0.62
1:C:168:ARG:NH2	1:C:170:ASP:OD1	2.32	0.61
2:F:1:DA:H1'	2:F:2:DC:C6	2.36	0.61
1:A:184:ALA:O	1:A:186:ARG:N	2.34	0.61
1:D:188:ASP:O	1:D:191:SER:N	2.34	0.61
1:B:34:THR:N	1:B:36:GLU:OE1	2.34	0.60
1:B:69:PRO:HG2	1:B:73:ALA:HA	0.66	0.60
1:A:33:MET:CB	1:A:35:LEU:HA	2.31	0.60
1:C:52:ALA:HB2	1:C:93:TYR:HD1	1.67	0.60
1:A:169:LYS:O	1:A:172:LEU:N	2.35	0.60
1:D:35:LEU:HD22	1:D:139:SER:OG	2.03	0.59
1:B:71:ARG:O	1:B:72:SER:HB2	2.01	0.58
1:D:87:THR:OG1	1:D:99:ASP:OD1	2.17	0.58
1:D:96:ARG:HG2	1:D:133:ILE:HD13	1.84	0.58
1:B:40:ASN:OD1	1:B:41:GLU:N	2.37	0.58
1:C:104:GLU:CD	1:C:139:SER:HB3	2.29	0.58
1:D:96:ARG:NH1	1:D:131:ASP:HB3	2.19	0.58
1:A:183:TYR:CD2	1:A:184:ALA:N	2.72	0.57
1:C:109:THR:HB	2:H:5:DA:OP2	2.04	0.57
1:C:138:ILE:HD11	1:C:172:LEU:HD22	1.86	0.57
1:D:148:GLU:OE1	1:D:197:TYR:OH	2.21	0.57
1:D:104:GLU:C	1:D:104:GLU:CD	2.73	0.57
1:B:182:GLY:O	1:B:186:ARG:HA	2.05	0.57
1:C:34:THR:O	1:C:35:LEU:HB3	2.03	0.57
1:A:144:VAL:HG12	1:A:179:ILE:HD12	1.87	0.56
2:E:5:DA:H1'	2:E:6:DA:H5''	1.88	0.56
2:H:1:DA:H2''	2:H:2:DC:C5	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:NH2	1:A:164:ARG:HD3	2.20	0.56
1:D:69:PRO:C	1:D:73:ALA:HB3	2.29	0.56
2:E:2:DC:H2'	2:E:3:DG:C8	2.40	0.56
1:A:58:PRO:HD2	1:C:58:PRO:HD2	1.88	0.56
1:D:39:LEU:HA	1:D:42:THR:HG22	1.88	0.56
1:C:110:SER:CB	1:C:168:ARG:HA	2.35	0.55
1:A:34:THR:H	1:A:38:ASP:CB	2.19	0.55
1:A:33:MET:CB	1:A:35:LEU:CD1	2.84	0.55
1:D:28:TYR:CD1	1:D:28:TYR:N	2.73	0.55
1:D:69:PRO:CB	1:D:73:ALA:HB3	2.35	0.55
1:C:40:ASN:HA	1:C:43:ASN:HD22	1.72	0.55
1:C:89:TYR:O	1:C:90:ASN:HB3	2.06	0.55
1:D:174:GLU:OE1	1:D:174:GLU:N	2.37	0.55
1:B:69:PRO:CD	1:B:73:ALA:HA	2.29	0.55
1:A:148:GLU:OE2	1:A:197:TYR:OH	2.24	0.55
1:D:24:ARG:CB	1:D:25:ALA:CB	2.85	0.54
1:B:63:ILE:HD11	1:B:76:ILE:HG12	1.89	0.54
1:C:46:TYR:CZ	1:C:190:ILE:HB	2.41	0.54
1:A:123:HIS:HA	1:A:126:GLN:OE1	2.07	0.54
1:C:35:LEU:HD23	1:C:104:GLU:HB2	1.88	0.54
1:D:24:ARG:CB	1:D:25:ALA:CA	2.85	0.54
1:D:69:PRO:CD	1:D:73:ALA:HB3	2.38	0.54
1:B:131:ASP:OD1	1:B:131:ASP:O	2.26	0.54
1:C:98:ILE:HD12	1:C:133:ILE:HB	1.90	0.54
1:D:121:ILE:HD12	1:D:124:MET:HB2	1.89	0.54
1:D:171:GLU:OE1	1:D:171:GLU:N	2.39	0.54
1:C:184:ALA:HB3	1:C:185:PRO:CD	2.38	0.53
1:A:76:ILE:O	1:C:78:GLU:HA	2.08	0.53
1:D:186:ARG:O	1:D:186:ARG:CG	2.55	0.53
1:A:103:LYS:HB3	1:A:111:PHE:HZ	1.73	0.53
1:D:147:LEU:HD13	1:D:176:ALA:HB2	1.89	0.53
1:B:69:PRO:HG3	1:B:73:ALA:HA	1.72	0.53
1:A:39:LEU:C	1:A:43:ASN:ND2	2.64	0.53
1:D:69:PRO:CA	1:D:73:ALA:CB	2.87	0.53
1:A:123:HIS:O	1:A:124:MET:C	2.50	0.53
2:G:3:DG:H2''	2:G:4:DC:C6	2.44	0.53
1:D:69:PRO:O	1:D:73:ALA:CB	2.55	0.52
2:H:8:DT:H1'	2:H:9:DG:H5'	1.92	0.52
1:B:72:SER:N	1:B:73:ALA:HB2	2.24	0.52
2:E:3:DG:H1	2:F:10:DC:N4	2.08	0.52
1:B:145:TYR:HA	1:B:178:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:SER:HB2	1:D:167:ILE:O	2.09	0.52
1:B:53:VAL:HG23	1:D:130:GLN:HG3	1.91	0.52
1:B:56:LYS:HB2	1:B:89:TYR:CE2	2.45	0.51
1:A:39:LEU:C	1:A:43:ASN:HD21	2.19	0.51
1:B:188:ASP:O	1:B:191:SER:OG	2.28	0.51
1:D:96:ARG:HG3	1:D:97:TYR:N	2.24	0.51
1:D:151:LYS:O	1:D:155:PHE:HD1	1.93	0.51
1:D:194:GLU:HA	1:D:198:PHE:HD1	1.76	0.51
1:C:39:LEU:O	1:C:43:ASN:ND2	2.44	0.51
1:D:101:GLU:HB3	1:D:136:VAL:HG22	1.93	0.51
1:B:69:PRO:CD	1:B:73:ALA:CA	2.87	0.51
1:C:189:TYR:HA	1:C:192:ILE:HD13	1.92	0.51
1:A:128:LYS:HZ2	1:A:134:CYS:H	1.57	0.50
2:H:2:DC:H2''	2:H:3:DG:C8	2.46	0.50
1:D:35:LEU:HD12	1:D:38:ASP:HB2	1.93	0.50
1:D:146:PHE:N	1:D:177:TYR:O	2.43	0.50
2:G:11:DG:O6	2:H:2:DC:N4	2.39	0.50
1:B:123:HIS:HA	1:B:126:GLN:HG3	1.94	0.50
1:A:167:ILE:HG23	1:A:171:GLU:HG3	1.93	0.50
1:C:45:TYR:CE2	1:C:184:ALA:HB1	2.46	0.50
1:C:83:GLN:OE1	1:C:119:HIS:NE2	2.45	0.50
1:A:141:PHE:CD1	1:A:141:PHE:N	2.73	0.50
1:D:35:LEU:CD2	1:D:139:SER:HB3	2.41	0.50
1:B:58:PRO:HG2	1:D:58:PRO:HD2	1.95	0.49
1:D:145:TYR:HA	1:D:178:PRO:HA	1.93	0.49
1:A:183:TYR:O	1:A:184:ALA:C	2.53	0.49
1:C:97:TYR:CE1	1:C:99:ASP:HB2	2.47	0.49
1:D:104:GLU:O	1:D:104:GLU:CD	2.54	0.49
1:D:164:ARG:C	1:D:166:SER:H	2.20	0.49
1:A:123:HIS:NE2	1:A:127:VAL:CG2	2.76	0.49
1:D:194:GLU:HA	1:D:198:PHE:CD1	2.47	0.49
1:B:86:THR:CG2	1:D:55:HIS:CD2	2.95	0.49
1:D:69:PRO:N	1:D:73:ALA:CB	2.71	0.49
1:A:123:HIS:NE2	1:A:127:VAL:HG21	2.27	0.49
1:C:45:TYR:CD1	1:C:45:TYR:C	2.91	0.49
1:A:32:GLY:CA	1:A:104:GLU:OE1	2.60	0.49
1:B:69:PRO:O	1:B:70:LYS:C	2.57	0.48
1:D:24:ARG:CB	1:D:25:ALA:HA	2.43	0.48
1:D:53:VAL:HB	1:D:92:ILE:HG22	1.95	0.48
2:F:11:DG:H2''	2:F:12:DT:O5'	2.13	0.48
1:D:39:LEU:O	1:D:42:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ILE:HD13	1:C:91:GLY:HA3	1.94	0.48
1:D:28:TYR:HB2	1:D:31:ARG:O	2.13	0.48
1:A:45:TYR:CD1	1:A:45:TYR:C	2.92	0.48
1:B:87:THR:HG22	1:B:120:GLN:HG2	1.96	0.48
1:A:157:ASP:HA	1:A:160:GLU:CB	2.44	0.48
1:C:67:HIS:NE2	1:C:69:PRO:HG3	2.29	0.48
1:D:96:ARG:HD2	1:D:131:ASP:O	2.14	0.48
1:B:69:PRO:CG	1:B:74:ALA:N	2.77	0.48
1:C:181:LEU:HA	1:C:186:ARG:O	2.14	0.48
1:B:101:GLU:CG	1:B:136:VAL:HG23	2.43	0.47
1:D:88:ASN:HB3	1:D:89:TYR:CD1	2.49	0.47
1:A:118:ASP:CG	1:A:119:HIS:N	2.72	0.47
1:C:85:SER:O	1:C:86:THR:C	2.54	0.47
1:B:69:PRO:CB	1:B:72:SER:O	2.62	0.47
1:D:35:LEU:CD2	1:D:139:SER:CB	2.91	0.47
1:D:35:LEU:O	1:D:39:LEU:N	2.33	0.47
1:D:35:LEU:O	1:D:36:GLU:C	2.54	0.47
1:D:36:GLU:OE2	1:D:56:LYS:HE2	2.15	0.47
1:D:141:PHE:O	1:D:141:PHE:CD1	2.68	0.47
1:A:56:LYS:HE3	1:A:89:TYR:CZ	2.49	0.47
1:B:101:GLU:HG3	1:B:136:VAL:HG23	1.97	0.47
1:D:133:ILE:O	1:D:133:ILE:HG22	2.15	0.47
2:E:1:DA:H2''	2:E:2:DC:C6	2.49	0.47
1:C:141:PHE:CZ	1:C:169:LYS:HA	2.49	0.46
2:E:10:DC:H2''	2:E:11:DG:H8	1.80	0.46
1:C:138:ILE:HG13	1:C:145:TYR:HB2	1.98	0.46
2:G:7:DT:H2''	2:G:8:DT:O4'	2.16	0.46
1:D:47:LEU:HD22	1:D:55:HIS:HE1	1.80	0.46
1:C:53:VAL:O	1:C:54:ILE:HD13	2.15	0.46
1:C:71:ARG:O	1:C:72:SER:C	2.56	0.46
1:A:184:ALA:O	1:A:185:PRO:C	2.55	0.46
1:D:124:MET:HE2	1:D:134:CYS:SG	2.53	0.46
1:B:113:LEU:HD21	1:B:167:ILE:CD1	2.46	0.46
1:B:160:GLU:C	1:B:162:ASN:H	2.24	0.46
1:B:69:PRO:CD	1:B:73:ALA:C	2.87	0.45
1:B:60:PRO:HD2	1:B:84:SER:HA	1.98	0.45
1:C:97:TYR:HE1	1:C:99:ASP:HB2	1.80	0.45
1:A:118:ASP:OD2	1:A:119:HIS:CE1	2.70	0.45
1:A:97:TYR:CE1	1:C:91:GLY:C	2.95	0.45
1:C:111:PHE:HA	1:C:112:PRO:HD3	1.68	0.45
1:D:167:ILE:HG23	1:D:171:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASP:OD2	1:A:119:HIS:CG	2.70	0.45
1:B:87:THR:OG1	1:B:99:ASP:OD1	2.34	0.45
1:D:113:LEU:HD13	1:D:167:ILE:HD12	1.99	0.45
1:A:126:GLN:O	1:A:129:ALA:HB3	2.17	0.45
1:A:34:THR:HA	1:A:35:LEU:HA	1.61	0.45
1:D:97:TYR:HE2	1:D:99:ASP:HB2	1.82	0.45
2:E:10:DC:H2''	2:E:11:DG:C8	2.52	0.45
2:F:1:DA:C4'	2:F:2:DC:H5'	2.47	0.45
1:D:155:PHE:HD2	1:D:167:ILE:CD1	2.30	0.45
1:B:131:ASP:O	1:B:131:ASP:CG	2.58	0.44
1:C:185:PRO:HD2	1:C:185:PRO:O	2.17	0.44
2:F:6:DA:H2'	2:F:6:DA:H5'	1.79	0.44
1:C:35:LEU:CD2	1:C:104:GLU:HB2	2.48	0.44
1:C:158:ARG:NH2	1:C:171:GLU:OE2	2.48	0.44
1:B:69:PRO:CG	1:B:73:ALA:C	2.88	0.44
1:C:105:THR:HB	1:C:111:PHE:HD1	1.82	0.44
1:D:117:HIS:O	1:D:121:ILE:HG22	2.17	0.44
1:B:103:LYS:HA	1:B:103:LYS:HD3	1.86	0.44
1:D:96:ARG:HH11	1:D:131:ASP:HB3	1.81	0.44
1:B:97:TYR:HE1	1:B:99:ASP:HB2	1.82	0.44
1:C:197:TYR:CD1	1:C:197:TYR:N	2.84	0.44
1:A:128:LYS:NZ	1:A:134:CYS:H	2.16	0.44
1:C:124:MET:HB2	1:C:134:CYS:SG	2.57	0.44
1:D:121:ILE:O	1:D:124:MET:N	2.51	0.44
1:D:182:GLY:O	1:D:184:ALA:HA	2.18	0.44
1:B:42:THR:HG21	1:B:187:ILE:O	2.18	0.43
1:B:150:ASP:HA	1:B:153:PHE:HB2	2.00	0.43
1:B:191:SER:O	1:B:195:GLN:HG3	2.17	0.43
1:C:60:PRO:HG2	1:C:84:SER:CB	2.44	0.43
1:A:37:ASP:O	1:A:38:ASP:C	2.61	0.43
1:A:118:ASP:CG	1:A:119:HIS:H	2.25	0.43
1:C:151:LYS:O	1:C:155:PHE:HD1	2.00	0.43
1:C:120:GLN:O	1:C:124:MET:HG2	2.18	0.43
1:D:159:LYS:HA	1:D:163:GLY:HA3	1.99	0.43
2:F:6:DA:C2	2:F:7:DT:C2	3.06	0.43
1:A:184:ALA:C	1:A:186:ARG:N	2.76	0.43
1:B:131:ASP:OD1	1:B:131:ASP:C	2.60	0.43
1:A:104:GLU:HB3	1:A:139:SER:HB3	2.00	0.43
1:B:195:GLN:O	1:B:199:SER:C	2.61	0.43
1:C:106:LYS:O	1:C:107:ASN:C	2.60	0.43
1:C:150:ASP:HA	1:C:153:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HD12	1:D:113:LEU:HA	1.79	0.43
2:F:1:DA:H2'	2:F:1:DA:P	2.59	0.43
2:F:5:DA:H1'	2:F:6:DA:H5''	1.99	0.43
1:A:57:LYS:HB3	1:A:57:LYS:HE3	1.66	0.43
1:B:73:ALA:O	1:B:74:ALA:HB3	2.18	0.43
1:C:126:GLN:O	1:C:129:ALA:HB3	2.18	0.43
1:A:39:LEU:N	1:A:39:LEU:HD12	2.33	0.43
1:D:31:ARG:HA	1:D:32:GLY:HA2	1.69	0.43
1:D:93:TYR:O	1:D:94:LYS:C	2.60	0.43
1:A:90:ASN:ND2	1:C:90:ASN:ND2	2.63	0.42
1:A:135:PHE:CD2	1:A:146:PHE:CD1	3.04	0.42
1:D:155:PHE:CD2	1:D:167:ILE:CD1	3.00	0.42
1:A:47:LEU:HD11	1:C:126:GLN:NE2	2.34	0.42
1:A:100:PHE:CE2	1:A:137:ILE:HD12	2.54	0.42
1:A:183:TYR:CG	1:A:184:ALA:N	2.88	0.42
1:A:88:ASN:OD1	1:A:103:LYS:NZ	2.51	0.42
1:A:124:MET:HB3	1:A:134:CYS:SG	2.60	0.42
1:A:133:ILE:HG21	1:A:193:ILE:HG23	2.02	0.42
1:A:40:ASN:CA	1:A:43:ASN:ND2	2.76	0.42
1:A:97:TYR:CE2	1:A:99:ASP:HB2	2.55	0.42
1:B:69:PRO:HG2	1:B:73:ALA:CB	2.42	0.42
2:F:10:DC:H1'	2:F:11:DG:H5'	2.02	0.42
1:B:185:PRO:O	1:B:185:PRO:CD	2.68	0.41
1:C:150:ASP:HA	1:C:153:PHE:CD2	2.54	0.41
1:A:103:LYS:HB3	1:A:111:PHE:CZ	2.52	0.41
1:B:103:LYS:NZ	1:B:115:ASN:O	2.36	0.41
1:B:114:GLN:HE22	2:E:7:DT:H2'	1.85	0.41
1:C:124:MET:HG2	1:C:124:MET:H	1.71	0.41
1:D:93:TYR:O	1:D:96:ARG:N	2.51	0.41
1:A:30:ASN:C	1:A:32:GLY:HA2	2.44	0.41
1:A:123:HIS:CD2	1:A:123:HIS:C	2.98	0.41
1:B:113:LEU:C	1:B:115:ASN:H	2.26	0.41
1:C:104:GLU:OE1	1:C:139:SER:HB3	2.20	0.41
1:D:155:PHE:HD2	1:D:167:ILE:HD13	1.80	0.41
1:A:72:SER:HA	1:A:73:ALA:HA	1.80	0.41
1:D:110:SER:HB2	1:D:167:ILE:C	2.45	0.41
1:D:155:PHE:O	1:D:158:ARG:N	2.53	0.41
1:B:61:VAL:HG12	1:B:62:GLN:C	2.46	0.41
1:A:138:ILE:HD12	1:A:138:ILE:N	2.34	0.41
1:C:117:HIS:HB2	1:C:119:HIS:CE1	2.55	0.41
2:E:1:DA:H2''	2:E:2:DC:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:C	1:A:27:SER:H	2.29	0.41
1:A:75:VAL:O	1:A:76:ILE:C	2.64	0.41
1:B:37:ASP:HA	1:B:40:ASN:ND2	2.36	0.41
1:C:33:MET:O	1:C:34:THR:HB	2.20	0.41
1:C:93:TYR:CE1	1:C:94:LYS:CG	3.01	0.40
1:C:151:LYS:H	1:C:151:LYS:HG2	1.64	0.40
1:A:52:ALA:HB2	1:A:93:TYR:HD1	1.86	0.40
1:A:93:TYR:OH	1:A:194:GLU:OE1	2.28	0.40
1:A:146:PHE:HB2	1:A:179:ILE:HD11	2.02	0.40
1:B:122:GLU:O	1:B:123:HIS:C	2.64	0.40
1:A:86:THR:HG23	1:A:123:HIS:HE1	1.80	0.40
1:A:121:ILE:CD1	1:A:152:LEU:HD21	2.51	0.40
1:A:169:LYS:O	1:A:171:GLU:N	2.55	0.40
2:F:7:DT:H2''	2:F:8:DT:O5'	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:THR:CG2	2:G:7:DT:OP2[7_445]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	175/199 (88%)	147 (84%)	23 (13%)	5 (3%)	3	24
1	B	164/199 (82%)	146 (89%)	16 (10%)	2 (1%)	10	42
1	C	172/199 (86%)	139 (81%)	32 (19%)	1 (1%)	21	56
1	D	197/199 (99%)	160 (81%)	34 (17%)	3 (2%)	8	37
All	All	708/796 (89%)	592 (84%)	105 (15%)	11 (2%)	7	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ALA
1	B	185	PRO
1	C	185	PRO
1	A	48	THR
1	B	69	PRO
1	A	129	ALA
1	A	150	ASP
1	A	185	PRO
1	D	187	ILE
1	D	185	PRO
1	D	167	ILE

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	115/181 (64%)	113 (98%)	2 (2%)	53	75
1	B	114/181 (63%)	111 (97%)	3 (3%)	40	69
1	C	108/181 (60%)	105 (97%)	3 (3%)	38	68
1	D	99/181 (55%)	96 (97%)	3 (3%)	36	66
All	All	436/724 (60%)	425 (98%)	11 (2%)	42	69

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	121	ILE
1	B	81	PHE
1	B	122	GLU
1	B	126	GLN
1	C	61	VAL
1	C	98	ILE
1	C	197	TYR
1	D	28	TYR

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Mol	Chain	Res	Type
1	D	51	ILE
1	D	121	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	90	ASN
1	A	123	HIS
1	B	88	ASN
1	B	114	GLN
1	B	143	GLN
1	C	49	ASN
1	C	50	GLN
1	D	55	HIS
1	D	143	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](#)

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 ⓘ

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	177/199 (88%)	0.64	22 (12%) 8 6	48, 67, 95, 146	9 (5%)
1	B	166/199 (83%)	0.66	11 (6%) 24 15	52, 71, 104, 117	0
1	C	174/199 (87%)	0.41	8 (4%) 37 23	50, 81, 98, 126	5 (2%)
1	D	199/199 (100%)	0.72	18 (9%) 15 10	48, 85, 115, 143	31 (15%)
2	E	12/12 (100%)	-0.22	0 100 100	59, 79, 112, 113	0
2	F	12/12 (100%)	-0.43	0 100 100	62, 78, 104, 111	0
2	G	11/12 (91%)	0.40	1 (9%) 15 9	111, 123, 152, 153	0
2	H	11/12 (91%)	0.55	1 (9%) 15 9	105, 123, 162, 163	0
All	All	762/844 (90%)	0.58	61 (8%) 18 12	48, 76, 113, 163	45 (5%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	GLU	6.0
1	A	37	ASP	5.9
1	A	33	MET	5.9
1	D	10	PHE	5.4
1	D	53	VAL	4.8
1	B	41	GLU	4.8
1	B	131	ASP	4.6
1	D	111	PHE	4.3
1	A	34	THR	4.3
1	A	32	GLY	3.9
1	A	31	ARG	3.9
1	A	187	ILE	3.9
1	B	189	TYR	3.8
1	A	38	ASP	3.8
1	D	29	SER	3.7
1	A	39	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	199	SER	3.4
1	D	110	SER	3.4
1	D	28	TYR	3.4
1	B	67	HIS	3.4
1	A	84	SER	3.4
1	D	114	GLN	3.4
1	A	30	ASN	3.3
1	D	9	THR	3.1
1	A	29	SER	3.1
1	D	135	PHE	3.0
1	B	84	SER	3.0
1	D	199	SER	2.9
1	C	38	ASP	2.8
1	C	37	ASP	2.8
1	C	116	PHE	2.8
2	H	1	DA	2.7
1	C	114	GLN	2.7
1	D	31	ARG	2.7
1	D	80	TYR	2.6
1	D	4	TYR	2.6
1	C	199	SER	2.6
1	C	107	ASN	2.6
1	D	54	ILE	2.5
1	A	199	SER	2.4
1	A	67	HIS	2.4
1	C	124	MET	2.4
1	B	132	GLY	2.3
1	B	183	TYR	2.3
1	A	60	PRO	2.3
1	A	183	TYR	2.2
1	A	189	TYR	2.2
1	D	27	SER	2.2
1	A	35	LEU	2.2
1	D	112	PRO	2.2
1	A	45	TYR	2.2
1	A	75	VAL	2.2
1	D	92	ILE	2.2
1	C	40	ASN	2.1
1	D	141	PHE	2.1
1	B	187	ILE	2.1
1	B	172	LEU	2.0
1	B	188	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	26	PRO	2.0
1	A	72	SER	2.0
2	G	12	DT	2.0

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.