



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:20 AM UTC

PDB ID : 8WVZ / pdb_00008wvz
EMDB ID : EMD-37880
Title : Structure of ADP-Form AsfvPrimPol Hexamer
Authors : Shi, T.H.; Guo, Y.Y.; Yan, R.H.
Deposited on : 2023-10-24
Resolution : 3.15 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

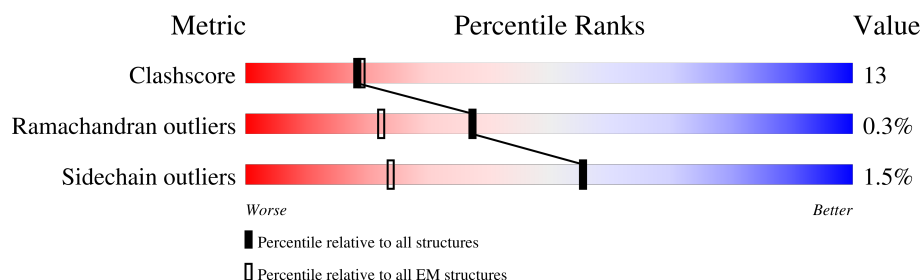
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	972	47% 18% . 34%
1	B	972	47% 19% . 34%
1	C	972	49% 16% . 34%
1	D	972	49% 17% . 34%
1	E	972	61% 28% . 10%
1	F	972	47% 18% . 34%
2	H	25	40% 60%
3	I	4	25% 75%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34621 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Putative primase C962R.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		
1	B	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		
1	C	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		
1	D	644	Total	C	N	O	S	0	0
			5333	3440	907	961	25		
1	E	874	Total	C	N	O	S	0	0
			7148	4605	1213	1300	30		
1	F	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	963	LEU	-	expression tag	UNP A0A2X0TKI6
A	964	GLU	-	expression tag	UNP A0A2X0TKI6
A	965	ASP	-	expression tag	UNP A0A2X0TKI6
A	966	TYR	-	expression tag	UNP A0A2X0TKI6
A	967	LYS	-	expression tag	UNP A0A2X0TKI6
A	968	ASP	-	expression tag	UNP A0A2X0TKI6
A	969	ASP	-	expression tag	UNP A0A2X0TKI6
A	970	ASP	-	expression tag	UNP A0A2X0TKI6
A	971	ASP	-	expression tag	UNP A0A2X0TKI6
A	972	LYS	-	expression tag	UNP A0A2X0TKI6
B	963	LEU	-	expression tag	UNP A0A2X0TKI6
B	964	GLU	-	expression tag	UNP A0A2X0TKI6
B	965	ASP	-	expression tag	UNP A0A2X0TKI6
B	966	TYR	-	expression tag	UNP A0A2X0TKI6
B	967	LYS	-	expression tag	UNP A0A2X0TKI6
B	968	ASP	-	expression tag	UNP A0A2X0TKI6
B	969	ASP	-	expression tag	UNP A0A2X0TKI6
B	970	ASP	-	expression tag	UNP A0A2X0TKI6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	971	ASP	-	expression tag	UNP A0A2X0TKI6
B	972	LYS	-	expression tag	UNP A0A2X0TKI6
C	963	LEU	-	expression tag	UNP A0A2X0TKI6
C	964	GLU	-	expression tag	UNP A0A2X0TKI6
C	965	ASP	-	expression tag	UNP A0A2X0TKI6
C	966	TYR	-	expression tag	UNP A0A2X0TKI6
C	967	LYS	-	expression tag	UNP A0A2X0TKI6
C	968	ASP	-	expression tag	UNP A0A2X0TKI6
C	969	ASP	-	expression tag	UNP A0A2X0TKI6
C	970	ASP	-	expression tag	UNP A0A2X0TKI6
C	971	ASP	-	expression tag	UNP A0A2X0TKI6
C	972	LYS	-	expression tag	UNP A0A2X0TKI6
D	963	LEU	-	expression tag	UNP A0A2X0TKI6
D	964	GLU	-	expression tag	UNP A0A2X0TKI6
D	965	ASP	-	expression tag	UNP A0A2X0TKI6
D	966	TYR	-	expression tag	UNP A0A2X0TKI6
D	967	LYS	-	expression tag	UNP A0A2X0TKI6
D	968	ASP	-	expression tag	UNP A0A2X0TKI6
D	969	ASP	-	expression tag	UNP A0A2X0TKI6
D	970	ASP	-	expression tag	UNP A0A2X0TKI6
D	971	ASP	-	expression tag	UNP A0A2X0TKI6
D	972	LYS	-	expression tag	UNP A0A2X0TKI6
E	963	LEU	-	expression tag	UNP A0A2X0TKI6
E	964	GLU	-	expression tag	UNP A0A2X0TKI6
E	965	ASP	-	expression tag	UNP A0A2X0TKI6
E	966	TYR	-	expression tag	UNP A0A2X0TKI6
E	967	LYS	-	expression tag	UNP A0A2X0TKI6
E	968	ASP	-	expression tag	UNP A0A2X0TKI6
E	969	ASP	-	expression tag	UNP A0A2X0TKI6
E	970	ASP	-	expression tag	UNP A0A2X0TKI6
E	971	ASP	-	expression tag	UNP A0A2X0TKI6
E	972	LYS	-	expression tag	UNP A0A2X0TKI6
F	963	LEU	-	expression tag	UNP A0A2X0TKI6
F	964	GLU	-	expression tag	UNP A0A2X0TKI6
F	965	ASP	-	expression tag	UNP A0A2X0TKI6
F	966	TYR	-	expression tag	UNP A0A2X0TKI6
F	967	LYS	-	expression tag	UNP A0A2X0TKI6
F	968	ASP	-	expression tag	UNP A0A2X0TKI6
F	969	ASP	-	expression tag	UNP A0A2X0TKI6
F	970	ASP	-	expression tag	UNP A0A2X0TKI6
F	971	ASP	-	expression tag	UNP A0A2X0TKI6
F	972	LYS	-	expression tag	UNP A0A2X0TKI6

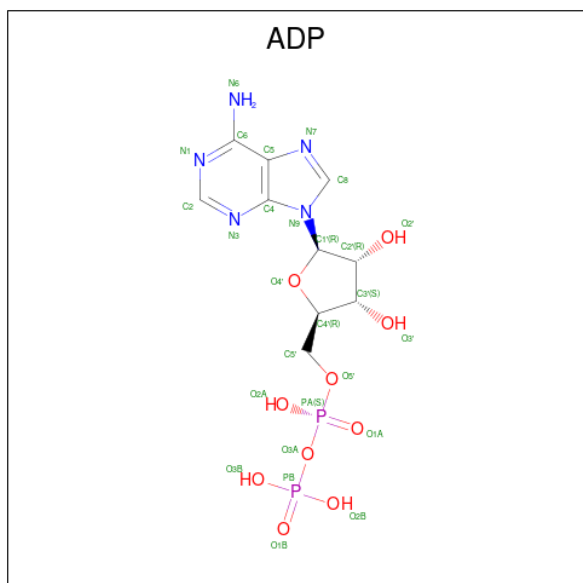
- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	25	Total	C	N	O	P	0	0
			500	250	50	175	25		

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	4	Total	C	N	O	P	0	0
			84	40	20	20	4		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

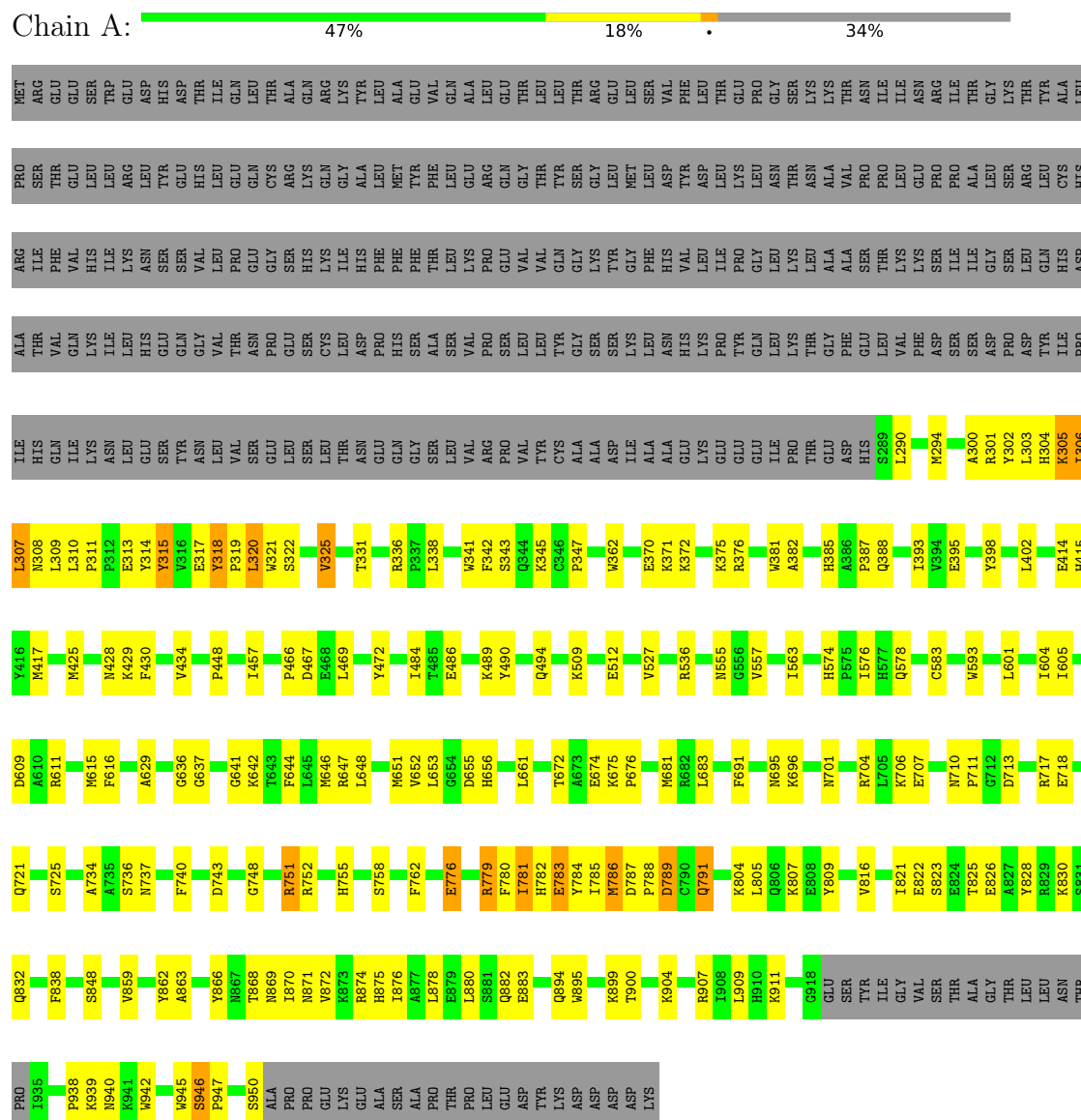
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Mg 1	0
5	B	1	Total 1	Mg 1	0
5	C	1	Total 1	Mg 1	0
5	D	1	Total 1	Mg 1	0
5	E	1	Total 1	Mg 1	0
5	F	1	Total 1	Mg 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

• Molecule 1: Putative primase C962R



• Molecule 1: Putative primase C962R

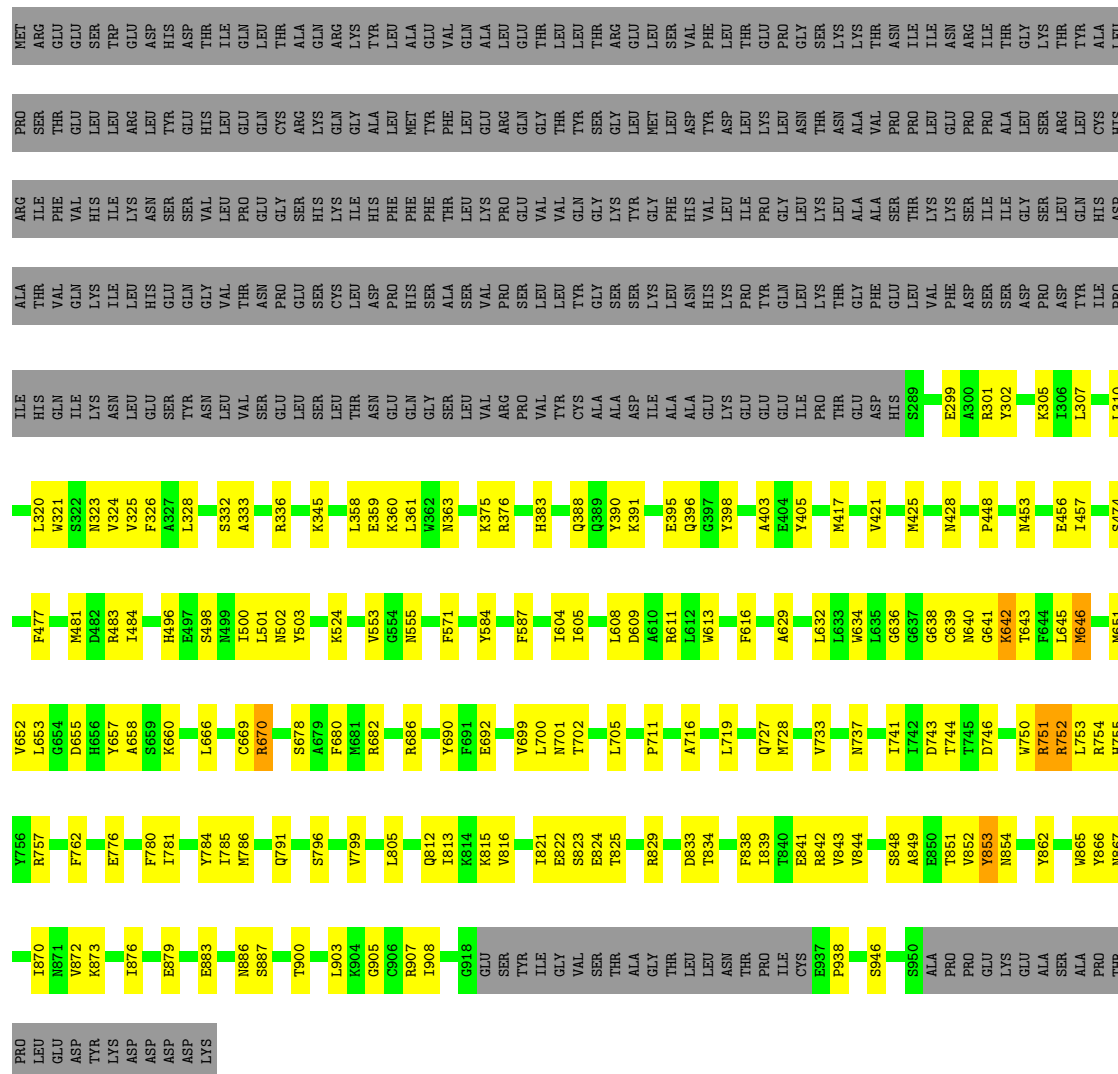


- Molecule 1: Putative primase C962R



● Molecule 1: Putative primase C962R

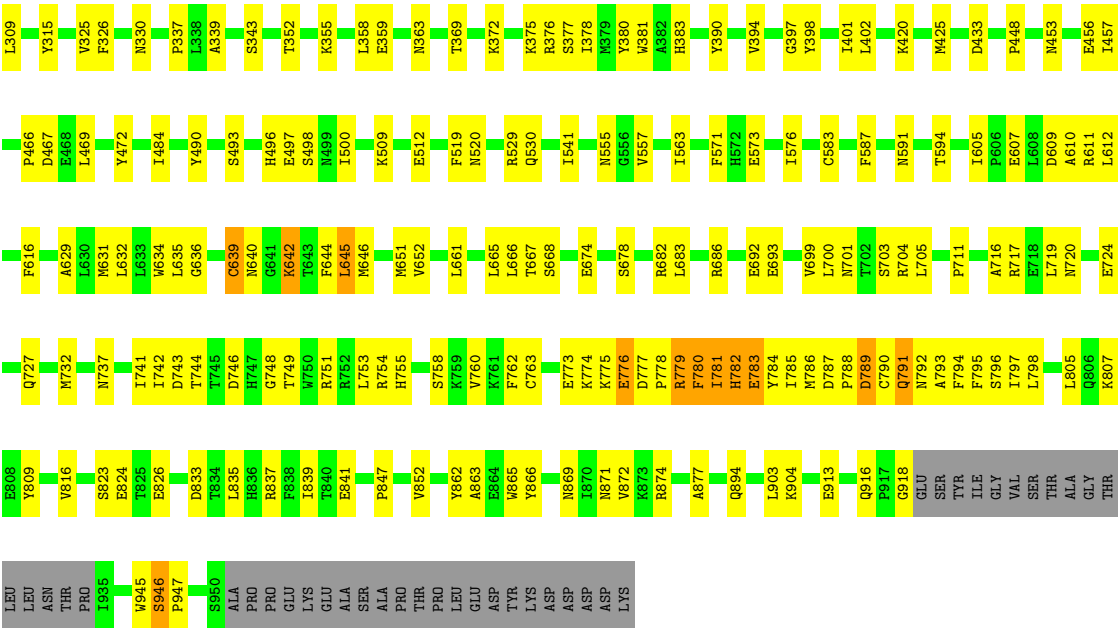
Chain D: 49% 17% 34%



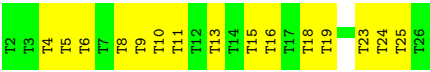
● Molecule 1: Putative primase C962R

GLU	W865	H747	K642	E359	ALA	L163	MET
ALA	Y866	G748	F643	Y490	ASP	L85	ARG
SER	N867	G749	F644	A365	ILE	L165	GLU
ALA	T868	T749	L645	Q494	ALA		SER
PRO	N869	Y750	M646	P495	GLU	K170	TRP
THR	T870	R751	R647	H496	LYS	K171	
PRO	N871	R752		E497	GLY	Y91	GLU
LEU	W872	L753	K660	S498	GLU	I174	ASP
GLU	K873	G754	S498	N499	GLY	G93	HIS
ASP	K874	H755	L665	I500	GLU	T182	ASP
TYR	H875	Y756		L501	ILE	L94	THR
LYS			S668		PRO	K185	ILE
ASP	L878	H764	C669	K505	THR		GLN
ASP	E879	D767	R670		GLU	H188	LEU
ASP	L890		E671	I518	ASP		THR
LYS			T672	Y390	HIS	Y192	ALA
	W895	K775	D521			T193	GLN
		E776	S522	V394	L290	N194	ARG
	R899	D777	F623	E395	S291	P107	TYR
	T900	P778	K524		T292	L199	LYS
	R901	R779	S678	Y398	L293	P109	LEU
		F780		V527	M294	L110	
	K904	I781	M881	T401	L295	E111	A22
	G905	H782	R882	L402	H296	P112	E23
	C906	E783	L883	R536	G297	P113	V24
	R907	Y784	K684	E404	P298	A114	L27
		I785		I541	E299	L115	
						G212	
	G916		M695	V553	A300	S116	L30
	PRO	Q791	K696	G411	R301		L31
GLY				N412	Y302	H120	
GLU	S796		N555		L303		E34
SER		V699	I563	H415	H304	F123	L35
TYR	Y809	S703	P564		K305		
ILE		R704		I418		K127	E41
GLY	V816	L705	N569	T422			
VAL		K706			N308	Q222	S44
SER	I821		F587		L309	L132	
THR	E822	P711		N428		PRO	I50
ALA	S823	ALA	I604		Y314	GLY	N51
GLY	E824	V714	I605	V432	Y315	GLY	R52
THR	T825			D433		SER	I53
LEU		R717	D609		L320	L229	
LEU	R837	E718	A610	W442	W321	V230	
ASN		L719	R611				P61
PRO	E841	N720	G611	L447	F326	P236	S62
THR		Q721	Y617	P448	A327	ASP	T63
ILE	A849	K722			L328	TYR	E64
	E850		G625	T457	A393	ILE	L65
CYS	E851	S725	L626		N330	PRO	L66
E937	Y852	F726	K627	L473		ILE	R67
	Y853		E628	S474	Y335	HIS	L68
K941		T729	A629	E475	R336	GLN	E70
			L630	N476	P337	ILE	Y69
	E857		M631	F477		LYS	E71
E944		W732		S478	E340	ASN	E73
				W479	W341	L247	
S950		A735	W634	V480	W350	F156	R76
ALA	T860	S736		N481		H157	K77
PRO		Y862	C639				
PRO		A863				T160	L81
GLU						CYS	P161
LYS		F864				ALA	C162

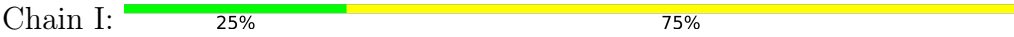
IIE	ALA	ARG	PRO	MET
HTS	THR	IIE	THR	ARG
GLN	VAL	PHE	SER	GLU
IIE	GLN	VAL	GLU	GLU
LYS	LYS	HIS	LEU	SER
ASN	IIE	IIE	LEU	TRP
GLU	LEU	LYS	ARG	GLU
GLU	HIS	ASN	LEU	ASP
SER	GLU	SER	TYR	HIS
TYR	GLN	SER	GLU	ASP
ASN	GLY	VAL	HIS	THR
LEU	VAL	LEU	LEU	IIE
VAL	THR	PRO	GLU	IIE
SER	ASN	GLU	GLN	LEU
GLU	PRO	GLY	CYS	THR
LEU	GLU	SER	ALA	GLU
SER	SER	HIS	LYS	GLN
LEU	CYS	LYS	GLN	ARG
THR	ASP	IIE	GLY	ARG
ASN	ASN	HIS	ALA	TYR
GLU	PRO	PHE	LEU	LEU
GLN	HIS	PHE	MET	ALA
GLY	SER	PHE	TYR	GLU
SER	ALA	THR	PHE	VAL
LEU	SER	LEU	LEU	GLN
VAL	VAL	LYS	GLU	ALA
ARG	PRO	PRO	ARG	LEU
PRO	SER	GLU	GLN	GLU
VAL	LEU	VAL	GLY	THR
TYR	LEU	VAL	THR	LEU
CYS	TYR	GLN	TYR	LEU
ALA	GLY	GLY	SER	THR
ALA	SER	LYS	GLY	THR
ASP	ASP	TYR	LEU	ARG
IIE	LYS	GLY	MET	GLU
ALA	LEU	PHE	LEU	LEU
ALA	ASN	HIS	ASP	SER
GLU	HIS	VAL	TYR	VAL
GLU	LYS	LEU	ASP	PHE
GLU	PRO	IIE	LEU	THR
GLU	TYR	PRO	LYS	THR
GLU	GLN	GLY	LEU	GLU
IIE	LEU	LEU	ASN	PRO
PRO	LYS	LYS	THR	GLY
THR	THR	LEU	ASN	SER
GLU	GLY	ALA	ALA	LYS
ASP	PHE	SER	VAL	THR
HIS	LEU	SER	PRO	ASN
IIE	GLU	THR	PRO	THR
L293	VAL	LYS	PRO	IIE
L293	PHE	LYS	LEU	ASN
P298	ASP	SER	PRO	ARG
E299	SER	IIE	PRO	ILE
A300	ASP	GLY	ALA	THR
Y302	ASP	SER	LEU	LYS
I306	TYR	GLN	LEU	THR
I306	IIE	HIS	CYS	ALA
I306	PRO	ASP	HTS	THR



● Molecule 2: DNA (25-MER)



● Molecule 3: DNA (5'-D(P*AP*AP*AP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101780	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.16	0/5503	0.37	0/7458
1	B	0.13	0/5503	0.35	0/7458
1	C	0.13	0/5503	0.34	1/7458 (0.0%)
1	D	0.14	0/5489	0.37	2/7439 (0.0%)
1	E	0.15	1/7341 (0.0%)	0.36	0/9948
1	F	0.22	0/5503	0.36	0/7458
2	H	0.20	0/549	0.51	0/846
3	I	0.11	0/95	0.16	0/144
All	All	0.16	1/35486 (0.0%)	0.36	3/48209 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	752	ARG	CA-C	-5.01	1.47	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	785	ILE	N-CA-C	-5.09	107.87	112.96
1	D	853	TYR	CA-C-N	5.05	131.18	121.54
1	D	853	TYR	C-N-CA	5.05	131.18	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5347	0	5217	169	0
1	B	5347	0	5217	142	0
1	C	5347	0	5217	136	0
1	D	5333	0	5201	125	0
1	E	7148	0	7053	199	0
1	F	5347	0	5217	136	0
2	H	500	0	301	14	0
3	I	84	0	45	4	0
4	A	27	0	12	4	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	4	0
4	E	27	0	12	2	0
4	F	27	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	34621	0	33540	892	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 13.

All (892) 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:751:ARG:HD3	1:A:752:ARG:NH1	1.81	0.95
1:A:748:GLY:HA2	1:A:751:ARG:HD2	1.49	0.92
1:F:779:ARG:HD3	1:F:783:GLU:HB2	1.52	0.92
1:F:376:ARG:HH12	1:F:571:PHE:HB3	1.36	0.89
1:F:644:PHE:HB2	1:F:781:ILE:HG12	1.54	0.89
1:A:751:ARG:HD3	1:A:752:ARG:HH11	1.34	0.89
1:A:647:ARG:HG3	1:A:785:ILE:HG21	1.55	0.87
1:D:751:ARG:HD2	1:D:752:ARG:HG3	1.57	0.85
1:A:779:ARG:HE	1:A:783:GLU:HB2	1.43	0.83
1:F:298:PRO:HA	1:F:301:ARG:HD3	1.60	0.81
1:E:748:GLY:HA2	1:E:751:ARG:HD2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:640:ASN:HD22	1:F:642:LYS:HG2	1.45	0.78
1:B:777:ASP:HB3	1:B:780:PHE:HB2	1.67	0.77
1:E:870:ILE:HA	1:F:877:ALA:HB3	1.67	0.77
1:A:604:ILE:HG13	4:A:1001:ADP:HN61	1.49	0.77
1:B:842:ARG:HE	1:B:909:LEU:HB2	1.49	0.77
1:F:852:VAL:HG21	1:F:903:LEU:HB3	1.67	0.76
1:E:383:HIS:HD1	1:E:390:TYR:HH	1.33	0.76
1:A:302:TYR:HA	1:A:305:LYS:HD2	1.67	0.76
1:A:648:LEU:HD13	1:A:785:ILE:HA	1.68	0.76
1:F:913:GLU:HG3	1:F:916:GLN:HE22	1.52	0.74
1:D:752:ARG:HH11	1:D:752:ARG:HG2	1.53	0.74
1:B:681:MET:SD	1:B:684:LYS:NZ	2.61	0.73
1:D:842:ARG:HH22	1:D:908:ILE:HG13	1.53	0.73
1:B:863:ALA:HA	1:B:866:TYR:CE2	2.24	0.73
1:C:681:MET:HA	1:C:684:LYS:HZ3	1.51	0.73
1:B:644:PHE:HE1	1:B:785:ILE:HD11	1.51	0.72
1:A:748:GLY:CA	1:A:751:ARG:HD2	2.18	0.72
1:B:639:CYS:HB2	1:B:762:PHE:HB2	1.72	0.72
1:C:695:ASN:ND2	1:D:701:ASN:O	2.23	0.71
1:A:652:VAL:HG22	1:A:791:GLN:HG3	1.72	0.71
1:B:640:ASN:HB3	1:B:642:LYS:HG3	1.72	0.71
1:A:370:GLU:HG2	1:A:372:LYS:H	1.56	0.70
1:C:370:GLU:H	1:C:372:LYS:HZ3	1.37	0.70
1:E:402:LEU:HD22	1:E:484:ILE:HG13	1.73	0.69
1:A:434:VAL:HG22	1:A:536:ARG:HH12	1.58	0.69
1:C:701:ASN:ND2	1:C:743:ASP:O	2.24	0.69
1:E:383:HIS:ND1	1:E:390:TYR:OH	2.23	0.69
1:D:781:ILE:HD12	4:D:1001:ADP:H5'1	1.75	0.69
1:E:365:ALA:O	1:E:368:HIS:ND1	2.25	0.69
1:E:866:TYR:HA	1:E:869:ASN:HB3	1.74	0.69
1:D:821:ILE:O	1:D:822:GLU:HG3	1.94	0.68
1:A:304:HIS:HA	1:A:307:LEU:HD23	1.75	0.68
1:A:648:LEU:HA	1:A:785:ILE:HG23	1.74	0.68
1:C:681:MET:HE3	1:C:718:GLU:HG3	1.76	0.68
1:E:298:PRO:HA	1:E:301:ARG:HG2	1.76	0.68
1:A:578:GLN:HE21	1:A:656:HIS:HB3	1.59	0.67
1:E:863:ALA:HA	1:E:866:TYR:CZ	2.29	0.67
1:A:311:PRO:HD3	1:A:385:HIS:CE1	2.30	0.67
1:A:779:ARG:HA	1:A:782:HIS:HB3	1.76	0.67
1:F:748:GLY:HA2	1:F:751:ARG:HD3	1.76	0.66
1:B:376:ARG:NH1	1:B:427:GLY:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:ARG:HH22	1:F:872:VAL:H	1.43	0.66
1:C:604:ILE:HG22	1:C:605:ILE:HG23	1.78	0.66
1:F:781:ILE:HG13	4:F:1001:ADP:H3'	1.76	0.66
1:D:325:VAL:HG21	1:D:358:LEU:HD11	1.77	0.65
1:F:701:ASN:ND2	1:F:743:ASP:O	2.30	0.65
1:E:677:ASN:H	1:E:717:ARG:HG2	1.61	0.65
1:D:376:ARG:NH2	1:D:428:ASN:O	2.30	0.65
1:D:762:PHE:HB3	1:D:776:GLU:HG3	1.79	0.65
1:F:668:SER:HB2	1:F:703:SER:HB2	1.79	0.65
1:C:375:LYS:HA	1:C:378:ILE:HD13	1.79	0.65
1:E:139:ILE:N	1:E:229:LEU:O	2.30	0.65
1:E:448:PRO:HG3	1:E:457:ILE:HD11	1.79	0.65
1:E:668:SER:H	1:E:703:SER:HB2	1.62	0.65
1:A:315:TYR:HE2	1:A:343:SER:HA	1.61	0.64
1:E:315:TYR:O	1:E:321:TRP:NE1	2.30	0.64
1:E:785:ILE:O	1:E:791:GLN:NE2	2.30	0.64
1:F:605:ILE:O	1:F:611:ARG:NH1	2.30	0.64
1:E:365:ALA:HA	1:E:368:HIS:HB3	1.79	0.64
1:A:681:MET:HG2	1:A:718:GLU:HG2	1.78	0.64
1:B:307:LEU:HD11	1:B:341:TRP:HZ3	1.63	0.64
1:F:711:PRO:O	1:F:727:GLN:NE2	2.31	0.64
1:F:652:VAL:HG21	1:F:794:PHE:HD2	1.63	0.63
1:B:894:GLN:HB3	1:B:904:LYS:HE3	1.79	0.63
1:D:842:ARG:HG3	1:D:843:VAL:HG23	1.79	0.63
1:C:706:LYS:O	1:C:710:ASN:ND2	2.31	0.63
1:B:318:TYR:HA	1:B:321:TRP:NE1	2.14	0.63
1:E:521:ASP:OD2	1:F:529:ARG:NH1	2.32	0.63
1:D:653:LEU:HD23	1:D:658:ALA:HB2	1.79	0.63
1:C:676:PRO:HB3	1:C:717:ARG:HG3	1.81	0.63
1:D:605:ILE:O	1:D:611:ARG:NH1	2.32	0.63
1:C:291:SER:O	1:C:295:LEU:HB2	1.99	0.62
1:E:111:GLU:HB3	1:E:113:PRO:HD2	1.81	0.62
1:A:870:ILE:HG23	1:B:878:LEU:HD11	1.82	0.62
1:D:711:PRO:O	1:D:727:GLN:NE2	2.33	0.62
1:A:866:TYR:OH	1:A:875:HIS:HD2	1.82	0.62
1:C:946:SER:HB2	1:C:950:SER:HA	1.82	0.62
1:D:307:LEU:HA	1:D:310:LEU:HD23	1.81	0.62
1:D:702:THR:HA	1:D:705:LEU:HB3	1.80	0.62
1:E:85:LEU:HD23	1:E:209:LEU:HB3	1.82	0.62
1:C:309:LEU:HD22	1:C:389:GLN:HG3	1.82	0.62
1:D:660:LYS:NZ	1:D:692:GLU:OE2	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:VAL:HG11	1:A:576:ILE:HG21	1.82	0.62
1:B:870:ILE:HA	1:C:877:ALA:HB2	1.82	0.61
1:A:303:LEU:O	1:A:306:ILE:HG12	1.99	0.61
1:A:331:THR:HG21	1:A:375:LYS:HD3	1.82	0.61
1:D:376:ARG:CZ	1:D:428:ASN:HB2	2.30	0.61
1:D:750:TRP:CG	1:D:829:ARG:HD2	2.35	0.61
1:E:174:ILE:HD12	1:E:199:LEU:HD21	1.82	0.61
1:C:448:PRO:HG3	1:C:457:ILE:HD11	1.82	0.61
1:F:632:LEU:HG	1:F:634:TRP:HD1	1.66	0.61
2:H:24:DT:O4	3:I:2:DA:N6	2.34	0.61
1:E:477:PHE:O	1:E:481:MET:HG2	2.01	0.61
1:E:747:HIS:HD2	1:E:751:ARG:CZ	2.14	0.61
1:D:812:GLN:HB3	1:D:815:LYS:HG3	1.82	0.61
1:C:785:ILE:O	1:C:791:GLN:NE2	2.22	0.61
1:C:852:VAL:HG11	1:C:903:LEU:HB3	1.83	0.61
1:A:593:TRP:CD1	1:A:789:ASP:HB2	2.36	0.60
1:B:672:THR:OG1	1:B:704:ARG:NH2	2.33	0.60
1:B:676:PRO:HB3	1:B:718:GLU:HA	1.83	0.60
1:D:678:SER:HB3	1:D:719:LEU:HB2	1.82	0.60
1:E:521:ASP:OD1	1:F:530:GLN:NE2	2.32	0.60
1:A:672:THR:O	1:A:704:ARG:NH1	2.33	0.60
1:E:330:ASN:ND2	1:E:373:ILE:O	2.34	0.60
1:A:704:ARG:HA	1:A:707:GLU:HG3	1.83	0.60
1:F:557:VAL:HG11	1:F:576:ILE:HG21	1.83	0.60
1:A:448:PRO:HG3	1:A:457:ILE:HD11	1.82	0.60
1:E:88:GLN:OE1	1:E:170:LYS:NZ	2.33	0.60
1:C:490:TYR:O	1:C:494:GLN:NE2	2.35	0.60
1:C:562:THR:OG1	1:C:566:LYS:NZ	2.33	0.60
1:C:767:ASP:H	1:C:773:GLU:HG2	1.65	0.60
1:E:94:LEU:HB2	1:E:160:ILE:HB	1.83	0.60
1:D:307:LEU:HD21	1:D:345:LYS:HE2	1.84	0.60
1:D:604:ILE:HG22	1:D:605:ILE:HG23	1.83	0.60
1:A:402:LEU:HD22	1:A:484:ILE:HG13	1.83	0.60
1:A:636:GLY:HA3	1:A:758:SER:HB3	1.83	0.60
1:E:866:TYR:HA	1:E:869:ASN:CB	2.31	0.60
1:F:448:PRO:HG3	1:F:457:ILE:HD11	1.83	0.60
1:F:631:MET:HB3	1:F:753:LEU:HD23	1.82	0.60
1:C:740:PHE:O	1:C:832:GLN:NE2	2.34	0.60
1:A:848:SER:O	1:A:907:ARG:NH2	2.33	0.60
1:C:290:LEU:HG	1:C:294:MET:HE1	1.83	0.60
1:E:350:TRP:O	1:E:355:LYS:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:629:ALA:HB2	1:F:711:PRO:HD3	1.84	0.59
1:D:785:ILE:O	1:D:791:GLN:NE2	2.31	0.59
1:B:895:TRP:HA	1:B:901:ARG:HA	1.84	0.59
1:E:678:SER:HB3	1:E:719:LEU:HD23	1.84	0.59
1:A:604:ILE:HG22	1:A:605:ILE:HG23	1.84	0.59
1:A:637:GLY:O	1:A:737:ASN:ND2	2.35	0.59
1:E:98:TYR:HE1	1:E:199:LEU:HD12	1.68	0.59
1:F:762:PHE:HB3	1:F:776:GLU:HG3	1.84	0.59
1:B:639:CYS:CB	1:B:762:PHE:HB2	2.32	0.59
1:C:863:ALA:HA	1:C:866:TYR:CD2	2.38	0.59
1:B:448:PRO:HG3	1:B:457:ILE:HD11	1.85	0.59
1:C:946:SER:HB3	1:C:947:PRO:HD2	1.85	0.59
1:B:834:THR:HB	1:B:865:TRP:HZ3	1.68	0.59
1:A:707:GLU:HA	1:A:710:ASN:HD21	1.68	0.58
1:E:604:ILE:HG22	1:E:605:ILE:HG23	1.84	0.58
1:F:299:GLU:HA	1:F:302:TYR:CE1	2.38	0.58
1:A:317:GLU:CG	1:A:320:LEU:HB2	2.34	0.58
1:B:764:HIS:O	1:B:775:LYS:NZ	2.37	0.58
1:D:646:MET:HE3	1:D:690:TYR:HD2	1.67	0.58
1:E:748:GLY:HA2	1:E:751:ARG:CD	2.33	0.58
1:E:91:TYR:HB2	1:E:164:LYS:HB2	1.84	0.58
1:B:911:LYS:HG3	1:B:912:PHE:H	1.69	0.58
1:E:81:LEU:O	1:E:82:MET:HE2	2.04	0.58
1:A:911:LYS:NZ	1:B:856:SER:OG	2.36	0.58
1:A:675:LYS:HB2	1:A:676:PRO:HD3	1.86	0.58
1:E:328:LEU:HA	1:E:375:LYS:HZ3	1.69	0.58
1:F:402:LEU:HD22	1:F:484:ILE:HG13	1.86	0.58
1:E:300:ALA:HA	1:E:303:LEU:HD12	1.86	0.58
1:A:302:TYR:O	1:A:306:ILE:HG23	2.04	0.57
1:C:395:GLU:HA	1:C:398:TYR:CZ	2.39	0.57
1:E:30:LEU:HD11	1:E:67:ARG:HH21	1.67	0.57
1:E:145:LEU:HD22	1:E:224:LYS:HE3	1.85	0.57
1:F:555:ASN:ND2	1:F:583:CYS:SG	2.76	0.57
1:B:376:ARG:CZ	1:B:428:ASN:HA	2.33	0.57
1:F:398:TYR:CZ	1:F:425:MET:HG3	2.39	0.57
1:B:852:VAL:HG11	1:B:903:LEU:HB3	1.86	0.57
1:E:105:ASN:HA	1:E:153:LYS:HD3	1.85	0.57
1:E:634:TRP:HB3	1:E:756:TYR:HB3	1.85	0.57
1:F:674:GLU:O	1:F:717:ARG:NH1	2.38	0.57
1:D:502:ASN:OD1	1:D:503:TYR:N	2.36	0.57
1:E:326:PHE:O	1:E:330:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:750:TRP:CD2	1:D:829:ARG:HD2	2.38	0.57
1:F:795:PHE:O	1:F:796:SER:C	2.47	0.57
1:E:123:PHE:O	1:E:127:LYS:HG2	2.04	0.57
1:E:660:LYS:O	1:E:682:ARG:NH2	2.37	0.57
1:E:755:HIS:ND1	1:E:824:GLU:OE1	2.38	0.57
1:F:720:ASN:HD21	2:H:8:DT:H4'	1.70	0.57
1:A:740:PHE:O	1:A:832:GLN:NE2	2.38	0.57
1:F:788:PRO:O	1:F:789:ASP:C	2.48	0.57
1:A:490:TYR:O	1:A:494:GLN:NE2	2.37	0.57
1:B:375:LYS:O	1:B:376:ARG:HB2	2.03	0.57
1:E:192:VAL:HG12	1:E:194:ASN:H	1.69	0.57
1:F:779:ARG:C	1:F:783:GLU:HB3	2.30	0.57
1:B:863:ALA:O	1:B:867:ASN:HB3	2.04	0.57
1:C:854:ASN:H	1:C:902:ILE:HG13	1.70	0.57
1:E:31:LEU:HD23	1:E:35:LEU:HD13	1.87	0.57
1:A:318:TYR:N	1:A:319:PRO:HD2	2.21	0.56
1:A:415:HIS:HA	1:A:527:VAL:HG22	1.86	0.56
1:C:378:ILE:HA	1:C:381:TRP:HE3	1.69	0.56
1:C:636:GLY:HA3	1:C:640:ASN:CG	2.30	0.56
1:F:793:ALA:O	1:F:794:PHE:C	2.47	0.56
1:A:701:ASN:ND2	1:A:743:ASP:O	2.39	0.56
1:B:444:GLU:OE2	1:B:461:ARG:NE	2.38	0.56
1:B:644:PHE:CD1	1:B:781:ILE:HG12	2.40	0.56
1:B:834:THR:OG1	1:B:862:TYR:OH	2.23	0.56
1:D:388:GLN:OE1	1:D:391:LYS:NZ	2.35	0.56
1:F:837:ARG:O	1:F:841:GLU:HB3	2.05	0.56
1:B:840:THR:HA	1:B:844:VAL:HB	1.87	0.56
1:E:672:THR:O	1:E:704:ARG:NH1	2.38	0.56
1:E:821:ILE:HG23	1:E:822:GLU:OE1	2.05	0.56
1:F:791:GLN:O	1:F:792:ASN:C	2.48	0.56
1:C:718:GLU:O	1:C:721:GLN:NE2	2.39	0.56
1:D:359:GLU:OE1	1:D:360:LYS:NZ	2.39	0.56
1:A:290:LEU:O	1:A:294:MET:HG2	2.05	0.55
1:C:838:PHE:HB2	1:C:865:TRP:CZ3	2.40	0.55
1:E:30:LEU:HD12	1:E:34:GLU:HB2	1.87	0.55
1:A:706:LYS:O	1:A:710:ASN:ND2	2.39	0.55
1:D:780:PHE:HA	1:D:784:TYR:HD2	1.72	0.55
1:F:376:ARG:O	1:F:376:ARG:HD3	2.05	0.55
1:A:317:GLU:HG3	1:A:320:LEU:HB2	1.88	0.55
1:A:821:ILE:O	1:A:822:GLU:HG3	2.07	0.55
1:E:76:ARG:HD2	1:E:212:GLY:HA3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:ILE:HG13	1:F:871:ASN:HD21	1.71	0.55
1:D:751:ARG:CZ	1:D:752:ARG:NH2	2.70	0.55
1:F:753:LEU:O	1:F:754:ARG:NH1	2.37	0.55
1:D:453:ASN:N	1:D:456:GLU:OE2	2.39	0.55
1:E:292:ILE:HA	1:E:295:LEU:HG	1.87	0.55
1:A:578:GLN:NE2	1:A:656:HIS:O	2.40	0.55
1:D:752:ARG:HG2	1:D:752:ARG:NH1	2.21	0.55
1:E:563:ILE:HD12	1:E:564:PRO:HA	1.87	0.55
1:E:605:ILE:O	1:E:611:ARG:NH1	2.40	0.55
1:E:629:ALA:HB2	1:E:711:PRO:HD3	1.88	0.55
1:B:438:GLY:O	1:B:439:LYS:HD2	2.06	0.54
1:D:498:SER:HA	1:D:501:LEU:HD13	1.88	0.54
1:E:747:HIS:HD2	1:E:751:ARG:NE	2.05	0.54
1:A:555:ASN:ND2	1:A:583:CYS:SG	2.80	0.54
1:C:644:PHE:HE1	1:C:785:ILE:HD11	1.72	0.54
1:E:301:ARG:O	1:E:304:HIS:ND1	2.40	0.54
1:E:617:TYR:OH	1:E:732:MET:O	2.24	0.54
1:C:634:TRP:CZ2	1:C:642:LYS:HB3	2.43	0.54
1:A:804:LYS:HE2	1:A:945:TRP:HB2	1.90	0.54
1:C:878:LEU:O	1:C:882:GLN:NE2	2.36	0.54
1:A:303:LEU:HD11	1:A:338:LEU:HD11	1.89	0.54
1:C:675:LYS:NZ	2:H:4:DT:O2	2.39	0.54
1:E:301:ARG:HA	1:E:304:HIS:ND1	2.23	0.54
1:B:849:ALA:HB3	1:B:907:ARG:HB2	1.90	0.54
1:C:834:THR:OG1	1:C:862:TYR:OH	2.26	0.54
1:D:376:ARG:CZ	1:D:571:PHE:HZ	2.20	0.54
1:F:863:ALA:HA	1:F:866:TYR:CZ	2.42	0.54
1:C:370:GLU:N	1:C:372:LYS:HZ3	2.06	0.54
1:C:818:CYS:HB3	1:C:821:ILE:HG22	1.90	0.54
1:D:604:ILE:HD11	4:D:1001:ADP:N7	2.23	0.54
1:F:667:THR:HG22	1:F:700:LEU:HB3	1.90	0.54
1:E:146:LYS:HG3	1:E:154:TYR:HA	1.90	0.54
1:E:640:ASN:N	4:E:1001:ADP:O2B	2.41	0.54
1:E:665:LEU:O	1:E:704:ARG:NE	2.33	0.54
1:F:794:PHE:HA	1:F:797:ILE:HD12	1.90	0.53
1:A:755:HIS:HB3	1:A:825:THR:HA	1.91	0.53
1:B:608:LEU:HD22	1:B:938:PRO:HD3	1.90	0.53
1:C:639:CYS:SG	1:C:762:PHE:HB2	2.48	0.53
1:E:490:TYR:O	1:E:494:GLN:NE2	2.42	0.53
1:F:661:LEU:HD12	1:F:732:MET:HE1	1.91	0.53
1:C:821:ILE:O	1:C:822:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TYR:CD1	1:A:315:TYR:C	2.87	0.53
1:B:319:PRO:O	1:B:323:ASN:ND2	2.42	0.53
1:C:330:ASN:CG	1:C:372:LYS:HA	2.33	0.53
1:C:884:LEU:O	1:C:887:SER:OG	2.21	0.53
1:F:466:PRO:HB2	1:F:469:LEU:HB3	1.90	0.53
1:B:719:LEU:HG	2:H:6:DT:H3'	1.89	0.53
1:B:739:ASN:HD21	1:C:878:LEU:HD11	1.74	0.53
1:E:418:ILE:HD12	1:E:523:PHE:HE2	1.72	0.53
1:A:644:PHE:HA	1:A:785:ILE:HD11	1.91	0.53
1:A:876:ILE:HA	1:F:871:ASN:HD21	1.72	0.53
1:B:849:ALA:HB1	1:B:907:ARG:HH21	1.73	0.53
1:C:863:ALA:HA	1:C:866:TYR:CE2	2.43	0.53
1:A:804:LYS:HZ1	1:A:945:TRP:CD1	2.25	0.53
1:B:946:SER:HB3	1:B:947:PRO:HD2	1.90	0.53
1:C:374:THR:HG23	1:C:376:ARG:HB3	1.90	0.53
1:D:608:LEU:HD22	1:D:938:PRO:HD3	1.91	0.53
1:B:899:LYS:HE2	1:B:899:LYS:HA	1.91	0.53
1:F:678:SER:HB2	1:F:719:LEU:HD21	1.91	0.53
1:A:381:TRP:O	1:A:385:HIS:ND1	2.40	0.53
1:A:629:ALA:HB2	1:A:711:PRO:HD3	1.91	0.53
1:B:809:TYR:CE2	1:B:815:LYS:HB2	2.44	0.53
1:B:946:SER:HB2	1:B:950:SER:HA	1.91	0.53
1:C:640:ASN:HB3	1:C:642:LYS:HG3	1.91	0.53
1:E:587:PHE:HA	1:E:796:SER:HB3	1.91	0.53
1:F:862:TYR:CD1	1:F:866:TYR:HE2	2.27	0.53
1:E:609:ASP:OD1	1:E:609:ASP:N	2.41	0.53
1:B:605:ILE:O	1:B:611:ARG:NH1	2.42	0.52
1:A:859:VAL:HG22	1:A:880:LEU:HB2	1.92	0.52
1:D:746:ASP:OD1	1:D:746:ASP:N	2.40	0.52
1:A:695:ASN:HB3	1:B:703:SER:HB3	1.91	0.52
1:B:631:MET:HB3	1:B:753:LEU:HD23	1.90	0.52
2:H:25:DT:O4	3:I:1:DA:N6	2.43	0.52
1:C:297:ASP:HB3	1:C:300:ALA:CB	2.39	0.52
1:D:839:ILE:HG23	1:D:843:VAL:HB	1.91	0.52
2:H:23:DT:O4	3:I:3:DA:N6	2.42	0.52
1:A:387:PRO:O	1:A:388:GLN:HG3	2.10	0.52
1:A:946:SER:HB3	1:A:947:PRO:HD2	1.92	0.52
1:C:631:MET:HE2	1:C:631:MET:HA	1.92	0.52
1:A:414:GLU:OE2	1:F:520:ASN:HA	2.09	0.52
1:B:672:THR:H	1:B:704:ARG:HH21	1.58	0.52
1:E:107:VAL:O	1:E:109:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:794:PHE:O	1:F:795:PHE:C	2.51	0.52
1:B:844:VAL:HG12	1:B:845:GLU:HG3	1.92	0.52
1:E:863:ALA:HA	1:E:866:TYR:CE2	2.45	0.52
1:A:563:ILE:HD13	1:A:807:LYS:HG2	1.92	0.52
1:B:864:GLU:HA	1:B:867:ASN:HD22	1.75	0.52
1:D:682:ARG:O	1:D:686:ARG:NE	2.42	0.52
1:D:866:TYR:HE2	1:D:873:LYS:HG2	1.75	0.52
1:E:717:ARG:NE	1:E:721:GLN:O	2.43	0.52
1:F:636:GLY:HA2	1:F:758:SER:HB3	1.91	0.52
1:A:644:PHE:HB2	1:A:781:ILE:HG13	1.92	0.51
1:A:661:LEU:HD11	1:A:683:LEU:HD11	1.91	0.51
1:A:863:ALA:HA	1:A:866:TYR:CE2	2.44	0.51
1:A:866:TYR:HA	1:A:869:ASN:HB3	1.91	0.51
1:B:317:GLU:HG2	1:B:319:PRO:HD2	1.92	0.51
1:D:641:GLY:HA2	4:D:1001:ADP:O5'	2.10	0.51
1:E:93:GLY:HA3	1:E:161:PRO:HA	1.93	0.51
1:D:328:LEU:HD13	1:D:375:LYS:HZ2	1.76	0.51
1:D:883:GLU:O	1:D:887:SER:N	2.44	0.51
1:C:413:LEU:HB3	1:C:418:ILE:HD11	1.92	0.51
1:D:642:LYS:HG3	4:D:1001:ADP:O3B	2.10	0.51
1:D:903:LEU:HD23	1:D:905:GLY:H	1.75	0.51
1:E:671:GLU:HB3	1:E:675:LYS:HE3	1.91	0.51
1:F:616:PHE:HB3	1:F:805:LEU:HD12	1.91	0.51
1:F:783:GLU:HG2	1:F:784:TYR:N	2.24	0.51
1:A:467:ASP:N	1:A:467:ASP:OD1	2.42	0.51
1:F:755:HIS:ND1	1:F:824:GLU:OE1	2.44	0.51
1:B:700:LEU:HD13	1:B:740:PHE:HB3	1.93	0.51
1:F:790:CYS:O	1:F:791:GLN:C	2.53	0.51
1:A:713:ASP:OD1	1:A:725:SER:OG	2.28	0.51
1:B:303:LEU:HA	1:B:306:ILE:HG12	1.92	0.51
1:D:728:MET:SD	1:D:728:MET:N	2.83	0.51
1:E:162:GLY:O	1:E:269:VAL:N	2.42	0.51
1:E:647:ARG:HH21	1:E:781:ILE:HD11	1.76	0.51
1:D:477:PHE:O	1:D:481:MET:HG2	2.10	0.51
1:E:415:HIS:HA	1:E:527:VAL:HG12	1.93	0.51
1:A:804:LYS:HZ1	1:A:945:TRP:CG	2.29	0.51
1:C:892:TYR:O	1:C:904:LYS:N	2.40	0.51
1:D:395:GLU:HA	1:D:398:TYR:CE1	2.45	0.51
1:C:643:THR:HA	1:C:646:MET:HE2	1.93	0.51
1:E:304:HIS:HB2	1:E:341:TRP:HZ3	1.76	0.51
1:E:714:VAL:HG23	1:E:726:PHE:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ARG:CG	1:A:785:ILE:HG21	2.37	0.50
1:D:359:GLU:OE2	1:D:363:ASN:ND2	2.42	0.50
1:F:782:HIS:H	1:F:782:HIS:CD2	2.29	0.50
1:B:647:ARG:O	1:B:651:MET:HG2	2.11	0.50
1:B:680:PHE:C	1:B:681:MET:HE2	2.37	0.50
1:C:780:PHE:HA	1:C:784:TYR:HD2	1.76	0.50
1:C:609:ASP:OD1	1:C:609:ASP:N	2.44	0.50
1:C:639:CYS:O	1:C:762:PHE:HD1	1.94	0.50
1:D:854:ASN:HD22	1:D:900:THR:HG22	1.76	0.50
1:C:893:LEU:HA	1:C:903:LEU:HA	1.93	0.50
1:A:748:GLY:HA2	1:A:751:ARG:CD	2.33	0.50
1:B:381:TRP:HA	1:B:384:LYS:HE3	1.94	0.50
1:E:867:ASN:HA	1:E:871:ASN:O	2.12	0.50
1:F:775:LYS:HZ3	1:F:776:GLU:H	1.58	0.50
1:C:777:ASP:HB3	1:C:780:PHE:HB2	1.93	0.50
1:D:838:PHE:O	1:D:841:GLU:HG3	2.11	0.50
1:A:780:PHE:O	1:A:784:TYR:HB2	2.12	0.50
1:B:336:ARG:HE	1:B:340:GLU:HG2	1.76	0.50
1:C:309:LEU:O	1:C:385:HIS:NE2	2.43	0.50
1:D:813:ILE:O	1:D:816:VAL:HG12	2.11	0.50
1:F:847:PRO:HD2	1:F:918:GLY:HA3	1.92	0.50
2:H:10:DT:H2''	2:H:11:DT:O5'	2.12	0.50
1:F:563:ILE:HD13	1:F:807:LYS:HG3	1.94	0.49
1:B:520:ASN:ND2	1:C:414:GLU:OE2	2.45	0.49
1:E:822:GLU:HA	1:E:825:THR:HB	1.94	0.49
1:E:851:THR:OG1	1:E:907:ARG:NH1	2.46	0.49
1:F:716:ALA:N	1:F:724:GLU:O	2.44	0.49
1:A:425:MET:SD	1:A:472:TYR:OH	2.62	0.49
1:E:422:ILE:HG13	1:E:473:ILE:HG22	1.93	0.49
1:A:782:HIS:HE1	1:B:626:LEU:HG	1.78	0.49
1:A:309:LEU:HD11	1:A:393:ILE:HG13	1.95	0.49
1:A:876:ILE:HG23	1:A:878:LEU:HG	1.94	0.49
1:A:642:LYS:NZ	1:A:736:SER:O	2.46	0.49
1:B:681:MET:HE3	1:B:718:GLU:OE2	2.12	0.49
1:D:395:GLU:HA	1:D:398:TYR:CZ	2.47	0.49
1:E:51:ASN:HD21	1:E:53:ILE:HD12	1.78	0.49
1:B:325:VAL:HA	1:B:328:LEU:HG	1.95	0.49
1:D:396:GLN:OE1	1:D:483:ARG:NH2	2.43	0.49
1:E:24:VAL:HA	1:E:27:LEU:HD13	1.93	0.49
1:A:429:LYS:HB3	1:A:430:PHE:CD1	2.48	0.49
1:B:822:GLU:HA	1:B:825:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:867:ASN:HA	1:C:871:ASN:O	2.12	0.49
1:E:433:ASP:OD1	1:E:536:ARG:NH1	2.43	0.49
1:E:695:ASN:OD1	1:E:696:LYS:N	2.45	0.49
1:A:314:TYR:CD1	1:A:320:LEU:HG	2.48	0.49
1:C:639:CYS:HB2	1:C:761:LYS:HD2	1.95	0.49
1:E:777:ASP:HB3	1:E:780:PHE:HB2	1.95	0.49
1:D:652:VAL:HG22	1:D:791:GLN:HG3	1.95	0.48
1:D:699:VAL:HA	1:D:741:ILE:HB	1.94	0.48
1:F:743:ASP:OD1	1:F:743:ASP:N	2.44	0.48
1:A:787:ASP:HB3	1:A:789:ASP:OD2	2.13	0.48
1:D:834:THR:OG1	1:D:862:TYR:OH	2.25	0.48
1:E:305:LYS:O	1:E:309:LEU:HG	2.12	0.48
1:E:432:VAL:HG23	1:E:536:ARG:HA	1.95	0.48
1:E:752:ARG:O	1:E:753:LEU:HG	2.13	0.48
1:D:448:PRO:HG3	1:D:457:ILE:HD11	1.94	0.48
1:E:107:VAL:HG12	1:E:148:GLU:HG2	1.96	0.48
1:E:837:ARG:O	1:E:841:GLU:HB3	2.13	0.48
1:F:425:MET:HE3	1:F:472:TYR:HE1	1.78	0.48
1:B:665:LEU:HD21	1:B:679:ALA:HB1	1.94	0.48
1:D:553:VAL:HG23	1:D:555:ASN:H	1.79	0.48
1:D:822:GLU:HA	1:D:825:THR:HB	1.94	0.48
1:E:376:ARG:HD2	1:E:428:ASN:HB2	1.95	0.48
1:E:837:ARG:O	1:E:841:GLU:CB	2.61	0.48
1:D:821:ILE:C	1:D:823:SER:H	2.22	0.48
1:E:764:HIS:HA	1:E:775:LYS:HD2	1.96	0.48
1:A:616:PHE:HZ	1:A:804:LYS:HZ2	1.60	0.48
1:A:895:TRP:HB2	1:A:899:LYS:HA	1.94	0.48
1:C:631:MET:HB3	1:C:753:LEU:HD23	1.95	0.48
1:E:146:LYS:HD3	1:E:221:TYR:CE1	2.48	0.48
1:E:475:GLU:OE2	1:E:479:ARG:NH2	2.47	0.48
1:F:306:ILE:HA	1:F:309:LEU:HD12	1.94	0.48
1:F:837:ARG:O	1:F:841:GLU:CB	2.62	0.48
1:B:403:ALA:HA	1:B:406:VAL:HG12	1.95	0.48
1:B:609:ASP:OD1	1:B:609:ASP:N	2.45	0.48
1:B:867:ASN:ND2	1:B:868:THR:HG23	2.29	0.48
1:C:631:MET:HE1	1:C:732:MET:HB2	1.96	0.48
1:C:821:ILE:C	1:C:823:SER:H	2.21	0.48
1:C:859:VAL:HG22	1:C:880:LEU:HD23	1.95	0.48
1:D:328:LEU:HD22	1:D:375:LYS:HZ1	1.78	0.48
1:E:292:ILE:HB	1:E:296:HIS:CE1	2.48	0.48
1:C:367:HIS:O	1:C:367:HIS:ND1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:GLU:OE1	1:C:371:LYS:HE2	2.13	0.48
1:C:621:ALA:HB1	1:C:688:TYR:HB2	1.95	0.48
1:D:646:MET:HE1	1:D:692:GLU:HA	1.95	0.48
1:F:315:TYR:HE1	1:F:343:SER:HA	1.79	0.48
1:B:853:TYR:N	1:B:857:GLU:OE2	2.38	0.48
1:B:866:TYR:CD1	1:B:866:TYR:C	2.91	0.48
1:C:623:PHE:HB3	1:C:627:LYS:HE2	1.95	0.48
1:E:170:LYS:HE3	1:E:204:ALA:HB1	1.96	0.48
1:E:684:LYS:NZ	1:E:725:SER:O	2.45	0.48
1:A:787:ASP:H	1:A:791:GLN:HE22	1.62	0.48
1:B:311:PRO:HD2	1:B:314:TYR:CG	2.49	0.48
1:B:336:ARG:HH11	1:B:362:TRP:HD1	1.61	0.48
1:F:833:ASP:N	1:F:833:ASP:OD1	2.45	0.48
1:A:605:ILE:O	1:A:611:ARG:NH1	2.46	0.47
1:A:779:ARG:HH22	1:B:626:LEU:HD23	1.78	0.47
1:A:788:PRO:HA	1:A:791:GLN:HB2	1.96	0.47
1:A:823:SER:O	1:A:826:GLU:HG3	2.13	0.47
1:B:335:TYR:CD2	1:B:338:LEU:HD22	2.49	0.47
1:B:682:ARG:HH21	1:C:723:GLN:HB2	1.79	0.47
1:B:755:HIS:ND1	1:B:824:GLU:OE1	2.46	0.47
1:E:163:LEU:HD13	1:E:165:LEU:HD23	1.96	0.47
1:E:862:TYR:CE1	1:E:866:TYR:HD2	2.31	0.47
1:F:682:ARG:HA	1:F:682:ARG:HD3	1.71	0.47
1:A:938:PRO:HG3	1:A:942:TRP:HB3	1.95	0.47
1:C:292:ILE:O	1:C:296:HIS:ND1	2.45	0.47
1:C:297:ASP:HB3	1:C:300:ALA:HB2	1.96	0.47
1:C:299:GLU:HA	1:C:302:TYR:HB2	1.96	0.47
1:C:375:LYS:HZ2	1:C:379:MET:HB2	1.78	0.47
1:C:639:CYS:HB3	1:C:762:PHE:H	1.79	0.47
1:E:809:TYR:CZ	1:E:816:VAL:HG23	2.50	0.47
2:H:4:DT:H2"	2:H:5:DT:C6	2.49	0.47
1:A:784:TYR:O	1:A:785:ILE:C	2.56	0.47
1:B:359:GLU:OE1	1:B:363:ASN:ND2	2.46	0.47
1:B:779:ARG:NH1	1:B:784:TYR:OH	2.47	0.47
1:D:636:GLY:HA3	1:D:757:ARG:HG3	1.95	0.47
1:E:849:ALA:O	1:E:906:CYS:N	2.47	0.47
1:E:853:TYR:HB2	1:E:857:GLU:HG2	1.97	0.47
1:C:640:ASN:HB3	1:C:642:LYS:CG	2.44	0.47
1:D:336:ARG:HH12	1:D:359:GLU:HA	1.78	0.47
1:E:185:LYS:HA	1:E:188:HIS:HB2	1.97	0.47
1:B:320:LEU:HA	1:B:323:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:863:ALA:HB1	1:C:875:HIS:CE1	2.50	0.47
1:E:61:PRO:HD2	1:E:64:GLU:OE2	2.15	0.47
1:E:86:GLU:O	1:E:208:SER:N	2.45	0.47
1:F:375:LYS:HG3	1:F:376:ARG:H	1.79	0.47
1:A:641:GLY:HA2	4:A:1001:ADP:O1A	2.14	0.47
1:B:809:TYR:HE1	1:B:816:VAL:HG23	1.80	0.47
1:D:584:TYR:HE1	1:D:799:VAL:HG21	1.80	0.47
1:D:755:HIS:ND1	1:D:824:GLU:OE1	2.47	0.47
1:E:229:LEU:HG	1:E:230:VAL:H	1.80	0.47
1:E:518:ILE:O	1:E:524:LYS:NZ	2.38	0.47
1:F:352:THR:H	1:F:355:LYS:HZ3	1.61	0.47
1:F:789:ASP:O	1:F:790:CYS:C	2.58	0.47
1:F:795:PHE:O	1:F:798:LEU:N	2.47	0.47
1:B:863:ALA:HA	1:B:866:TYR:CD2	2.50	0.47
1:C:375:LYS:HB3	1:C:375:LYS:HE3	1.59	0.47
1:E:211:TYR:OH	1:E:223:LEU:N	2.48	0.47
1:F:496:HIS:HB2	1:F:500:ILE:HG23	1.97	0.47
1:B:681:MET:HE2	1:B:681:MET:N	2.29	0.47
1:D:634:TRP:CH2	1:D:642:LYS:HA	2.49	0.47
1:E:304:HIS:O	1:E:308:ASN:ND2	2.48	0.47
1:E:336:ARG:O	1:E:340:GLU:HG2	2.15	0.47
1:F:359:GLU:OE2	1:F:363:ASN:ND2	2.45	0.47
1:A:294:MET:HE3	1:A:301:ARG:HB3	1.97	0.47
1:A:609:ASP:N	1:A:609:ASP:OD1	2.46	0.47
1:A:646:MET:HE2	1:A:646:MET:N	2.30	0.47
1:B:290:LEU:HD12	1:B:293:LEU:HD12	1.96	0.47
1:B:672:THR:HG21	1:B:677:ASN:HD22	1.80	0.47
1:C:641:GLY:H	4:C:1001:ADP:PB	2.38	0.47
1:C:742:ILE:H	1:C:832:GLN:CD	2.23	0.47
1:D:751:ARG:HD2	1:D:752:ARG:CG	2.38	0.47
1:E:215:LYS:HB2	1:E:218:HIS:HB2	1.97	0.47
1:F:644:PHE:CD1	1:F:781:ILE:HA	2.50	0.47
1:A:414:GLU:OE1	1:F:519:PHE:HB3	2.16	0.46
1:B:627:LYS:NZ	1:B:729:THR:O	2.48	0.46
1:C:755:HIS:ND1	1:C:824:GLU:OE1	2.48	0.46
1:D:653:LEU:HG	1:D:657:TYR:HB2	1.96	0.46
1:D:838:PHE:HD1	1:D:865:TRP:CD2	2.33	0.46
1:E:859:VAL:HG22	1:E:880:LEU:HB3	1.97	0.46
1:A:307:LEU:HD13	1:A:342:PHE:CE1	2.50	0.46
1:A:776:GLU:HA	4:A:1001:ADP:H1'	1.97	0.46
1:B:809:TYR:CE1	1:B:816:VAL:HG23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:613:TRP:CH2	1:D:754:ARG:HD2	2.51	0.46
1:E:116:SER:O	1:E:120:HIS:ND1	2.48	0.46
1:F:293:LEU:HD11	1:F:337:PRO:HB2	1.98	0.46
2:H:9:DT:H2''	2:H:10:DT:H5''	1.97	0.46
1:B:331:THR:HG21	1:B:375:LYS:HB2	1.98	0.46
1:E:103:ASN:OD1	1:E:104:THR:N	2.49	0.46
1:F:782:HIS:CD2	1:F:782:HIS:N	2.84	0.46
1:A:644:PHE:HA	1:A:781:ILE:HG13	1.97	0.46
1:C:939:LYS:HG3	1:C:940:ASN:H	1.80	0.46
1:E:699:VAL:HA	1:E:741:ILE:HB	1.97	0.46
1:A:302:TYR:O	1:A:305:LYS:HG2	2.15	0.46
1:B:693:GLU:OE1	1:B:737:ASN:N	2.47	0.46
1:C:642:LYS:HE2	1:C:735:ALA:HB1	1.98	0.46
1:C:670:ARG:HH12	1:C:704:ARG:HG2	1.80	0.46
1:E:66:LEU:O	1:E:70:GLU:HG2	2.15	0.46
1:E:291:SER:OG	1:E:292:ILE:N	2.47	0.46
1:E:678:SER:O	1:E:681:MET:HG3	2.15	0.46
2:H:18:DT:H2'	2:H:19:DT:O4'	2.15	0.46
1:B:294:MET:HE1	1:B:301:ARG:HD2	1.97	0.46
1:B:395:GLU:HA	1:B:398:TYR:CE2	2.51	0.46
1:B:497:GLU:OE1	1:B:498:SER:N	2.49	0.46
1:C:640:ASN:N	4:C:1001:ADP:O2B	2.49	0.46
1:D:496:HIS:HB2	1:D:500:ILE:HG23	1.98	0.46
1:D:848:SER:OG	1:D:849:ALA:N	2.48	0.46
1:E:31:LEU:HA	1:E:35:LEU:HB3	1.98	0.46
1:A:783:GLU:O	1:A:785:ILE:N	2.48	0.46
1:B:651:MET:HE3	1:B:651:MET:HB3	1.89	0.46
1:D:320:LEU:HA	1:D:323:ASN:ND2	2.30	0.46
1:D:474:SER:HB2	1:D:524:LYS:NZ	2.31	0.46
1:E:753:LEU:O	1:E:754:ARG:NH1	2.41	0.46
1:B:866:TYR:HA	1:B:870:ILE:HG12	1.96	0.46
1:C:452:MET:HG2	1:C:453:ASN:O	2.16	0.46
1:D:299:GLU:HA	1:D:302:TYR:HD2	1.81	0.46
1:D:851:THR:OG1	1:D:907:ARG:NH1	2.49	0.46
1:E:395:GLU:HA	1:E:398:TYR:CE2	2.50	0.46
1:A:315:TYR:CE2	1:A:343:SER:HA	2.48	0.46
1:C:717:ARG:N	1:C:723:GLN:OE1	2.49	0.46
1:E:747:HIS:CD2	1:E:751:ARG:CZ	2.96	0.46
1:E:871:ASN:HD22	1:F:874:ARG:NH2	2.14	0.46
1:F:644:PHE:HD2	1:F:645:LEU:HD22	1.80	0.46
1:F:746:ASP:OD2	1:F:749:THR:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ALA:HB2	1:C:373:ILE:HB	1.98	0.46
1:C:373:ILE:H	1:C:373:ILE:HG12	1.51	0.46
1:D:587:PHE:HA	1:D:796:SER:HB3	1.97	0.46
1:E:671:GLU:HB2	1:E:675:LYS:HB2	1.97	0.46
1:F:378:ILE:HA	1:F:381:TRP:HD1	1.80	0.46
1:F:380:TYR:HA	1:F:383:HIS:HB3	1.98	0.46
1:F:809:TYR:CZ	1:F:816:VAL:HG23	2.51	0.46
1:D:833:ASP:OD1	1:D:833:ASP:N	2.45	0.45
1:E:41:GLU:HB3	1:E:44:SER:HB3	1.98	0.45
1:E:97:ASP:OD1	1:E:97:ASP:N	2.49	0.45
1:E:182:THR:O	1:E:185:LYS:HG3	2.16	0.45
1:E:862:TYR:O	1:E:865:TRP:HB3	2.16	0.45
1:F:786:MET:O	1:F:787:ASP:C	2.59	0.45
1:A:718:GLU:OE2	1:A:721:GLN:NE2	2.36	0.45
1:C:642:LYS:HG3	1:C:642:LYS:H	1.38	0.45
1:F:420:LYS:HB2	1:F:420:LYS:HE2	1.71	0.45
1:F:591:ASN:HB3	1:F:594:THR:HG23	1.99	0.45
1:A:809:TYR:CZ	1:A:816:VAL:HG23	2.51	0.45
1:A:907:ARG:HG2	1:A:909:LEU:HB2	1.97	0.45
1:C:557:VAL:HG11	1:C:576:ILE:HG21	1.99	0.45
1:E:627:LYS:NZ	1:E:729:THR:O	2.49	0.45
1:E:895:TRP:HB2	1:E:899:LYS:HA	1.98	0.45
1:F:339:ALA:O	1:F:343:SER:N	2.46	0.45
1:F:635:LEU:HD23	1:F:755:HIS:NE2	2.31	0.45
1:D:643:THR:HA	1:D:646:MET:SD	2.57	0.45
1:E:98:TYR:HD2	1:E:156:PHE:HB3	1.81	0.45
1:E:904:LYS:HD2	1:E:904:LYS:HA	1.75	0.45
1:F:467:ASP:OD1	1:F:467:ASP:N	2.49	0.45
1:F:612:LEU:HD13	1:F:945:TRP:HD1	1.81	0.45
1:F:823:SER:O	1:F:826:GLU:HG3	2.16	0.45
1:F:835:LEU:O	1:F:839:ILE:HG12	2.16	0.45
1:A:674:GLU:OE1	1:A:676:PRO:HD2	2.17	0.45
1:B:393:ILE:O	1:B:396:GLN:HG3	2.16	0.45
1:B:785:ILE:O	1:B:791:GLN:NE2	2.26	0.45
1:C:315:TYR:HA	1:C:321:TRP:HB2	1.97	0.45
1:C:646:MET:HE2	1:C:646:MET:HB2	1.75	0.45
1:E:50:ILE:O	1:E:85:LEU:N	2.46	0.45
1:F:326:PHE:O	1:F:330:ASN:ND2	2.47	0.45
1:F:394:VAL:HG22	1:F:398:TYR:CZ	2.51	0.45
1:F:453:ASN:N	1:F:456:GLU:OE2	2.38	0.45
1:F:497:GLU:OE1	1:F:498:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:640:ASN:HA	1:D:762:PHE:CD2	2.51	0.45
1:F:693:GLU:OE1	1:F:737:ASN:N	2.43	0.45
1:C:702:THR:HA	1:C:705:LEU:HB3	1.98	0.45
1:D:326:PHE:HE1	1:D:361:LEU:HB3	1.81	0.45
1:D:632:LEU:HB3	1:D:733:VAL:HG12	1.99	0.45
1:D:785:ILE:HG13	1:D:786:MET:SD	2.56	0.45
1:E:432:VAL:HG12	1:E:442:TRP:HA	1.99	0.45
1:A:305:LYS:HG2	1:A:306:ILE:N	2.32	0.45
1:A:899:LYS:O	1:A:900:THR:OG1	2.28	0.45
1:C:395:GLU:OE1	1:C:398:TYR:OH	2.31	0.45
1:F:783:GLU:O	1:F:784:TYR:HB2	2.16	0.45
1:E:866:TYR:O	1:E:870:ILE:HG12	2.16	0.45
1:B:492:LEU:HD12	1:B:504:TYR:HB3	1.99	0.45
1:B:652:VAL:HG21	1:B:794:PHE:HB3	1.98	0.45
1:E:703:SER:O	1:E:704:ARG:HG2	2.17	0.45
3:I:1:DA:H2"	3:I:2:DA:C8	2.52	0.45
1:A:307:LEU:HD13	1:A:342:PHE:CD1	2.53	0.44
1:A:322:SER:HA	1:A:325:VAL:HB	1.98	0.44
1:A:414:GLU:CD	1:A:415:HIS:N	2.75	0.44
1:A:644:PHE:CA	1:A:781:ILE:HG13	2.47	0.44
1:A:651:MET:HE1	1:A:786:MET:HA	1.99	0.44
1:C:659:SER:HB2	1:C:682:ARG:NH1	2.32	0.44
1:C:817:PHE:HZ	1:C:949:PRO:HA	1.81	0.44
1:E:226:GLY:H	1:E:247:LEU:HD11	1.82	0.44
1:E:941:LYS:O	1:E:944:GLU:HG2	2.17	0.44
1:A:382:ALA:HA	1:A:385:HIS:CE1	2.50	0.44
1:C:553:VAL:HG13	1:C:555:ASN:H	1.82	0.44
1:C:866:TYR:CD1	1:C:866:TYR:C	2.96	0.44
1:D:705:LEU:HD21	1:D:753:LEU:HD11	2.00	0.44
1:D:834:THR:HG21	1:D:870:ILE:HG13	2.00	0.44
1:E:153:LYS:HD2	1:E:153:LYS:HA	1.74	0.44
1:E:860:THR:O	1:E:864:GLU:OE1	2.36	0.44
1:E:906:CYS:SG	1:E:907:ARG:N	2.90	0.44
1:F:777:ASP:O	1:F:778:PRO:C	2.59	0.44
1:E:849:ALA:HB3	1:E:907:ARG:HB2	1.99	0.44
1:F:609:ASP:N	1:F:609:ASP:OD1	2.49	0.44
1:B:668:SER:OG	1:B:703:SER:O	2.25	0.44
1:B:821:ILE:C	1:B:823:SER:H	2.25	0.44
1:C:302:TYR:O	1:C:306:ILE:HG12	2.18	0.44
1:C:878:LEU:HD12	1:C:882:GLN:HG2	2.00	0.44
1:D:403:ALA:HA	1:D:484:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:779:ARG:O	1:E:783:GLU:HG3	2.16	0.44
2:H:4:DT:H4'	2:H:5:DT:OP1	2.16	0.44
1:C:892:TYR:HB2	1:C:903:LEU:HG	2.00	0.44
1:D:876:ILE:HG13	1:D:879:GLU:OE1	2.17	0.44
1:E:631:MET:HB3	1:E:753:LEU:HD23	1.99	0.44
1:F:865:TRP:O	1:F:869:ASN:HB2	2.17	0.44
1:B:853:TYR:O	1:B:902:ILE:HG12	2.18	0.44
1:F:784:TYR:O	1:F:785:ILE:C	2.60	0.44
1:D:323:ASN:OD1	1:D:324:VAL:N	2.51	0.44
1:D:616:PHE:HB3	1:D:805:LEU:HD12	1.98	0.44
1:D:883:GLU:HA	1:D:886:ASN:HB2	1.98	0.44
1:E:336:ARG:HB3	1:E:337:PRO:HD3	1.99	0.44
1:E:644:PHE:HA	1:E:781:ILE:HD13	2.00	0.44
1:C:487:HIS:CE1	1:C:491:HIS:CE1	3.05	0.44
1:D:834:THR:HG21	1:D:866:TYR:HD1	1.82	0.44
1:E:63:THR:O	1:E:66:LEU:HG	2.17	0.44
1:F:490:TYR:O	1:F:493:SER:OG	2.24	0.44
1:A:320:LEU:HD13	1:A:320:LEU:HA	1.83	0.44
1:A:466:PRO:HB2	1:A:469:LEU:HB3	2.00	0.44
1:B:404:GLU:OE2	1:B:408:SER:OG	2.33	0.44
1:D:481:MET:O	1:D:484:ILE:HG22	2.17	0.44
1:D:666:LEU:HB3	1:D:700:LEU:HD13	1.99	0.44
1:E:302:TYR:OH	1:E:394:VAL:HG12	2.18	0.44
1:F:587:PHE:HA	1:F:796:SER:HB3	2.00	0.44
1:A:395:GLU:HA	1:A:398:TYR:CE2	2.53	0.43
1:C:854:ASN:HA	1:C:902:ILE:HA	1.99	0.43
1:E:141:PHE:HE1	1:E:229:LEU:HB3	1.82	0.43
1:E:866:TYR:HE1	1:E:875:HIS:CE1	2.35	0.43
1:A:305:LYS:HG3	1:A:393:ILE:HG21	2.00	0.43
1:A:939:LYS:HG3	1:A:940:ASN:H	1.83	0.43
1:C:644:PHE:CE1	1:C:785:ILE:HD11	2.52	0.43
1:D:638:GLY:HA2	1:D:737:ASN:OD1	2.18	0.43
1:E:368:HIS:CD2	1:E:372:LYS:HE3	2.53	0.43
1:F:607:GLU:HB2	1:F:610:ALA:HB3	1.99	0.43
1:A:616:PHE:CD1	1:A:805:LEU:HB2	2.53	0.43
1:C:293:LEU:HD21	1:C:337:PRO:HB2	2.00	0.43
1:C:850:GLU:HA	1:C:905:GLY:HA2	2.00	0.43
1:D:651:MET:HE2	1:D:651:MET:HB2	1.84	0.43
1:E:65:LEU:O	1:E:68:LEU:HG	2.18	0.43
1:E:290:LEU:HG	1:E:294:MET:HG2	1.99	0.43
2:H:15:DT:H2''	2:H:16:DT:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:641:GLY:HA2	4:E:1001:ADP:O1A	2.18	0.43
1:F:783:GLU:C	1:F:785:ILE:H	2.26	0.43
1:B:666:LEU:HD12	1:B:705:LEU:HD12	2.00	0.43
1:C:375:LYS:O	1:C:376:ARG:C	2.61	0.43
1:D:328:LEU:HA	1:D:375:LYS:NZ	2.33	0.43
1:E:645:LEU:O	1:E:646:MET:C	2.62	0.43
1:A:838:PHE:CE2	1:A:862:TYR:HB2	2.54	0.43
1:A:882:GLN:N	1:A:882:GLN:OE1	2.51	0.43
1:B:509:LYS:O	1:B:512:GLU:HG3	2.18	0.43
1:B:776:GLU:HB3	4:B:1001:ADP:O2'	2.18	0.43
1:B:808:GLU:O	1:B:810:ASN:N	2.48	0.43
1:B:823:SER:O	1:B:826:GLU:HG3	2.18	0.43
1:B:899:LYS:HG3	1:B:900:THR:H	1.83	0.43
1:D:301:ARG:HB3	1:D:305:LYS:NZ	2.33	0.43
1:D:682:ARG:HD3	1:E:722:LYS:HG2	2.01	0.43
1:F:397:GLY:O	1:F:401:ILE:HG12	2.19	0.43
1:A:787:ASP:O	1:A:788:PRO:C	2.61	0.43
1:C:315:TYR:OH	1:C:343:SER:O	2.37	0.43
1:F:786:MET:HE3	1:F:786:MET:HB3	1.78	0.43
1:F:787:ASP:O	1:F:788:PRO:C	2.61	0.43
1:A:305:LYS:HE3	1:A:305:LYS:HB3	1.41	0.43
1:C:743:ASP:OD1	1:C:743:ASP:N	2.48	0.43
1:D:609:ASP:N	1:D:609:ASP:OD1	2.50	0.43
1:D:834:THR:HG21	1:D:866:TYR:CD1	2.54	0.43
1:D:867:ASN:HB3	1:D:872:VAL:HA	2.00	0.43
1:E:73:GLU:O	1:E:77:LYS:HG3	2.19	0.43
1:F:377:SER:OG	1:F:573:GLU:OE2	2.31	0.43
1:F:894:GLN:OE1	1:F:904:LYS:HG3	2.18	0.43
1:C:327:ALA:CB	1:C:373:ILE:HB	2.49	0.43
1:E:314:TYR:HA	1:E:320:LEU:HD13	2.00	0.43
1:E:873:LYS:HA	1:E:873:LYS:HD2	1.79	0.43
1:F:946:SER:HB3	1:F:947:PRO:HD2	2.00	0.43
1:A:313:GLU:CD	1:A:313:GLU:H	2.27	0.43
1:D:839:ILE:O	1:D:843:VAL:N	2.45	0.43
1:E:171:LYS:HD3	1:E:171:LYS:HA	1.73	0.43
1:E:395:GLU:OE1	1:E:398:TYR:OH	2.28	0.43
1:F:666:LEU:HD11	1:F:705:LEU:HD13	2.01	0.43
1:F:778:PRO:O	1:F:780:PHE:N	2.52	0.43
1:A:644:PHE:CE2	1:A:780:PHE:CZ	3.07	0.42
1:B:717:ARG:HB3	1:B:723:GLN:HG2	2.01	0.42
1:D:332:SER:OG	1:D:333:ALA:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:ARG:HA	1:A:782:HIS:CB	2.47	0.42
1:A:946:SER:HB2	1:A:950:SER:HA	2.01	0.42
1:B:376:ARG:HH22	1:B:460:TRP:HH2	1.66	0.42
1:C:378:ILE:O	1:C:379:MET:C	2.63	0.42
1:C:435:ASP:OD1	1:C:439:LYS:N	2.46	0.42
1:E:157:HIS:CD2	1:E:221:TYR:HE2	2.37	0.42
1:E:569:ASN:OD1	1:E:569:ASN:N	2.52	0.42
1:F:760:VAL:HG13	1:F:773:GLU:HA	2.00	0.42
1:A:786:MET:SD	1:A:786:MET:N	2.91	0.42
1:C:364:ASP:HA	1:C:367:HIS:CE1	2.55	0.42
1:F:383:HIS:ND1	1:F:390:TYR:OH	2.30	0.42
1:A:371:LYS:HE3	1:A:574:HIS:CD2	2.55	0.42
1:A:821:ILE:C	1:A:823:SER:H	2.27	0.42
1:B:395:GLU:OE1	1:B:398:TYR:OH	2.22	0.42
1:C:608:LEU:HD22	1:C:938:PRO:HD3	2.02	0.42
1:D:669:CYS:O	1:D:670:ARG:HD3	2.19	0.42
1:D:751:ARG:CZ	1:D:752:ARG:CZ	2.98	0.42
1:E:401:ILE:O	1:E:404:GLU:HG2	2.19	0.42
1:E:447:LEU:HG	1:E:448:PRO:HD2	2.01	0.42
1:A:417:MET:H	1:A:417:MET:HG2	1.70	0.42
1:A:601:LEU:HD11	1:A:615:MET:SD	2.59	0.42
1:C:361:LEU:HA	1:C:364:ASP:OD2	2.20	0.42
1:C:587:PHE:HA	1:C:796:SER:HB3	2.02	0.42
1:D:421:VAL:HG12	1:D:425:MET:HE3	1.99	0.42
1:D:744:THR:OG1	1:D:746:ASP:OD1	2.31	0.42
1:E:642:LYS:HE2	1:E:735:ALA:HB1	2.02	0.42
1:A:848:SER:OG	1:A:907:ARG:NH2	2.48	0.42
1:B:375:LYS:HG2	1:B:376:ARG:H	1.84	0.42
1:C:529:ARG:O	1:C:532:GLU:HG2	2.20	0.42
1:C:867:ASN:HD21	1:C:875:HIS:CE1	2.38	0.42
1:D:852:VAL:HG22	1:D:908:ILE:HD11	2.02	0.42
1:E:523:PHE:O	1:E:527:VAL:HG13	2.20	0.42
1:E:821:ILE:C	1:E:823:SER:H	2.28	0.42
1:A:740:PHE:O	1:A:828:TYR:OH	2.37	0.42
1:A:779:ARG:HA	1:A:779:ARG:HD2	1.74	0.42
1:A:883:GLU:OE1	1:A:883:GLU:N	2.51	0.42
1:B:635:LEU:HD23	1:B:755:HIS:HE2	1.84	0.42
1:B:640:ASN:HB3	1:B:642:LYS:CG	2.43	0.42
1:C:310:LEU:O	1:C:312:PRO:HD3	2.20	0.42
1:C:364:ASP:O	1:C:368:HIS:HB2	2.19	0.42
1:D:642:LYS:HG3	1:D:642:LYS:H	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:706:LYS:HA	1:E:706:LYS:HD3	1.81	0.42
1:A:822:GLU:HA	1:A:825:THR:HB	2.00	0.42
1:C:833:ASP:OD1	1:C:833:ASP:N	2.52	0.42
1:C:839:ILE:HA	1:C:843:VAL:HG22	2.01	0.42
1:D:680:PHE:CD2	1:D:716:ALA:HB3	2.54	0.42
1:D:870:ILE:HA	1:E:878:LEU:CD1	2.50	0.42
1:E:418:ILE:HD12	1:E:523:PHE:CE2	2.53	0.42
1:E:862:TYR:CE2	1:E:866:TYR:HE2	2.38	0.42
1:F:777:ASP:O	1:F:780:PHE:HB3	2.18	0.42
1:A:305:LYS:HA	1:A:308:ASN:ND2	2.34	0.42
1:A:336:ARG:HG3	1:A:362:TRP:NE1	2.35	0.42
1:A:429:LYS:HB3	1:A:430:PHE:CE1	2.54	0.42
1:B:336:ARG:HD2	1:B:362:TRP:CD1	2.54	0.42
1:B:635:LEU:HD11	1:B:739:ASN:HA	2.02	0.42
1:B:696:LYS:O	1:B:698:GLU:HG2	2.20	0.42
1:C:605:ILE:HA	1:C:606:PRO:HD3	1.85	0.42
1:C:783:GLU:O	1:C:784:TYR:HB2	2.20	0.42
1:E:309:LEU:HB3	1:E:389:GLN:NE2	2.35	0.42
1:E:941:LYS:HD3	1:E:941:LYS:HA	1.90	0.42
1:A:830:LYS:HD2	1:A:830:LYS:HA	1.83	0.42
1:B:378:ILE:HD12	1:B:378:ILE:H	1.85	0.42
1:C:426:MET:C	1:C:428:ASN:H	2.27	0.42
1:C:639:CYS:HB3	1:C:762:PHE:HB2	2.01	0.42
1:F:509:LYS:O	1:F:512:GLU:HG3	2.20	0.42
1:B:762:PHE:HB3	1:B:776:GLU:HG3	2.02	0.41
1:B:779:ARG:HB2	1:B:783:GLU:HG3	2.02	0.41
1:C:414:GLU:HG3	1:C:415:HIS:H	1.84	0.41
1:E:475:GLU:O	1:E:478:SER:OG	2.29	0.41
1:E:736:SER:OG	1:E:737:ASN:N	2.53	0.41
1:E:941:LYS:HD2	1:E:944:GLU:HB3	2.01	0.41
1:B:335:TYR:HD2	1:B:338:LEU:HD22	1.84	0.41
1:C:303:LEU:O	1:C:307:LEU:HG	2.19	0.41
1:C:681:MET:CE	1:C:718:GLU:HG3	2.48	0.41
1:D:669:CYS:C	1:D:670:ARG:HD3	2.45	0.41
1:E:497:GLU:OE2	1:E:499:ASN:HB3	2.20	0.41
1:A:311:PRO:HG2	1:A:314:TYR:CE1	2.56	0.41
1:A:341:TRP:O	1:A:345:LYS:NZ	2.53	0.41
1:A:466:PRO:HB2	1:A:469:LEU:CB	2.50	0.41
1:B:368:HIS:NE2	1:B:370:GLU:OE2	2.48	0.41
1:B:453:ASN:OD1	1:B:454:GLN:N	2.49	0.41
1:F:699:VAL:HA	1:F:741:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:DT:H6	2:H:13:DT:H2'	1.64	0.41
1:A:315:TYR:CE2	1:A:321:TRP:CZ2	3.08	0.41
1:B:481:MET:HE2	1:B:481:MET:HA	2.02	0.41
1:B:682:ARG:NH2	1:C:723:GLN:O	2.54	0.41
1:F:644:PHE:CE1	1:F:785:ILE:HD11	2.55	0.41
1:A:486:GLU:HA	1:A:489:LYS:HG2	2.02	0.41
1:A:876:ILE:HG13	1:F:871:ASN:ND2	2.35	0.41
1:B:763:CYS:N	1:B:776:GLU:OE2	2.53	0.41
1:B:809:TYR:CZ	1:B:815:LYS:HB2	2.56	0.41
1:B:892:TYR:HD2	1:B:904:LYS:HB2	1.85	0.41
1:D:853:TYR:O	1:D:854:ASN:OD1	2.38	0.41
1:E:328:LEU:HD12	1:E:335:TYR:HB3	2.02	0.41
1:E:336:ARG:NH1	1:E:359:GLU:OE1	2.54	0.41
1:E:476:ASN:O	1:E:480:VAL:HG23	2.20	0.41
1:E:864:GLU:HA	1:E:867:ASN:HB2	2.02	0.41
1:F:651:MET:HE2	1:F:651:MET:HB2	1.90	0.41
1:F:701:ASN:HD21	1:F:744:THR:HB	1.84	0.41
1:B:336:ARG:NE	1:B:340:GLU:HG2	2.35	0.41
1:D:834:THR:CG2	1:D:870:ILE:HG13	2.50	0.41
1:E:895:TRP:HB3	1:E:901:ARG:HA	2.03	0.41
1:F:398:TYR:CE2	1:F:425:MET:HG3	2.54	0.41
1:A:300:ALA:O	1:A:303:LEU:HG	2.21	0.41
1:A:376:ARG:NH1	1:A:428:ASN:HA	2.36	0.41
1:A:717:ARG:HD2	1:A:718:GLU:N	2.35	0.41
1:B:544:LEU:HD23	1:B:544:LEU:HA	1.96	0.41
1:C:439:LYS:N	1:C:439:LYS:HD3	2.36	0.41
1:E:368:HIS:CD2	1:E:372:LYS:HG2	2.55	0.41
1:F:369:THR:HA	1:F:372:LYS:NZ	2.36	0.41
1:F:742:ILE:HG22	1:F:744:THR:HG22	2.02	0.41
1:B:318:TYR:HA	1:B:321:TRP:HE1	1.85	0.41
1:B:601:LEU:HD23	1:B:942:TRP:HH2	1.86	0.41
1:B:783:GLU:OE1	1:B:784:TYR:N	2.53	0.41
1:B:818:CYS:HB3	1:B:821:ILE:HG22	2.02	0.41
1:C:742:ILE:HG22	1:C:744:THR:HG22	2.02	0.41
1:C:864:GLU:O	1:C:868:THR:HG22	2.21	0.41
1:E:410:ASN:HB3	1:E:412:MET:HE1	2.02	0.41
1:E:604:ILE:CD1	1:E:645:LEU:HD21	2.51	0.41
1:E:767:ASP:OD1	1:E:767:ASP:N	2.49	0.41
1:F:763:CYS:O	1:F:775:LYS:HA	2.21	0.41
2:H:5:DT:H2''	2:H:6:DT:C5	2.56	0.41
1:A:395:GLU:HA	1:A:398:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:LEU:HD23	1:A:653:LEU:HA	1.85	0.41
1:A:748:GLY:O	1:A:751:ARG:HD2	2.21	0.41
1:B:341:TRP:CH2	1:B:345:LYS:HD3	2.56	0.41
1:B:631:MET:SD	1:B:732:MET:HB2	2.61	0.41
1:B:641:GLY:H	4:B:1001:ADP:PB	2.43	0.41
1:B:653:LEU:HG	1:B:657:TYR:HB2	2.03	0.41
1:D:383:HIS:CD2	1:D:390:TYR:HH	2.39	0.41
1:D:655:ASP:OD1	1:D:655:ASP:C	2.64	0.41
1:E:110:LEU:HD23	1:E:115:LEU:HD21	2.02	0.41
1:E:496:HIS:HB2	1:E:500:ILE:HG23	2.01	0.41
1:E:501:LEU:O	1:E:505:LYS:HD2	2.21	0.41
1:E:553:VAL:HG13	1:E:555:ASN:H	1.86	0.41
1:E:642:LYS:HA	1:E:645:LEU:HD12	2.03	0.41
1:F:639:CYS:HA	4:F:1001:ADP:PA	2.61	0.41
1:A:306:ILE:HA	1:A:309:LEU:HD12	2.03	0.41
1:A:762:PHE:CZ	4:A:1001:ADP:C5	3.09	0.41
1:A:900:THR:HG22	1:F:841:GLU:HG3	2.03	0.41
1:B:778:PRO:O	1:B:782:HIS:ND1	2.52	0.41
1:D:321:TRP:CE2	1:D:358:LEU:HD13	2.56	0.41
1:D:358:LEU:HD12	1:D:358:LEU:HA	1.88	0.41
1:E:625:GLY:O	1:E:729:THR:OG1	2.35	0.41
1:F:325:VAL:HG21	1:F:358:LEU:HD21	2.02	0.41
1:B:682:ARG:HH22	1:C:722:LYS:HD3	1.86	0.40
1:D:405:TYR:HB3	1:D:417:MET:SD	2.61	0.40
1:E:52:ARG:HH22	1:E:215:LYS:HA	1.86	0.40
1:A:307:LEU:C	1:A:307:LEU:HD12	2.46	0.40
1:A:691:PHE:HB2	1:A:734:ALA:HA	2.02	0.40
1:A:871:ASN:CG	1:B:876:ILE:HG13	2.46	0.40
1:A:894:GLN:HB2	1:A:904:LYS:HD3	2.04	0.40
1:A:909:LEU:HD23	1:A:909:LEU:O	2.22	0.40
1:C:939:LYS:HG3	1:C:940:ASN:N	2.37	0.40
1:D:629:ALA:HB2	1:D:711:PRO:HD3	2.03	0.40
1:E:98:TYR:CD2	1:E:156:PHE:HB3	2.56	0.40
1:E:497:GLU:OE1	1:E:498:SER:N	2.54	0.40
1:E:706:LYS:HE3	1:E:749:THR:HG22	2.03	0.40
1:F:665:LEU:O	1:F:704:ARG:NH2	2.54	0.40
1:F:692:GLU:OE1	1:F:692:GLU:N	2.53	0.40
1:A:509:LYS:O	1:A:512:GLU:HG3	2.21	0.40
1:A:695:ASN:OD1	1:A:696:LYS:N	2.54	0.40
1:A:876:ILE:HA	1:F:871:ASN:ND2	2.36	0.40
1:B:780:PHE:HA	1:B:784:TYR:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:891:LYS:HG3	1:B:892:TYR:HD1	1.85	0.40
1:D:639:CYS:SG	1:D:762:PHE:HB2	2.61	0.40
1:D:743:ASP:OD1	1:D:743:ASP:N	2.54	0.40
1:F:775:LYS:NZ	1:F:776:GLU:H	2.18	0.40
1:A:655:ASP:OD1	1:A:656:HIS:N	2.54	0.40
1:B:311:PRO:HD3	1:B:385:HIS:CE1	2.57	0.40
1:B:336:ARG:NH1	1:B:362:TRP:HD1	2.19	0.40
1:B:496:HIS:CD2	1:B:499:ASN:HD21	2.40	0.40
1:B:653:LEU:HD23	1:B:658:ALA:HB2	2.03	0.40
1:B:744:THR:HG21	1:B:749:THR:HG21	2.03	0.40
1:D:854:ASN:HA	1:D:903:LEU:H	1.86	0.40
1:E:755:HIS:H	1:E:825:THR:HG1	1.67	0.40
1:F:433:ASP:HB3	1:F:541:ILE:HG12	2.03	0.40
1:F:683:LEU:HA	1:F:686:ARG:HB2	2.02	0.40
1:A:315:TYR:OH	1:A:347:PRO:HA	2.21	0.40
1:C:311:PRO:HD3	1:C:385:HIS:CE1	2.57	0.40
1:C:360:LYS:HD2	1:C:360:LYS:HA	1.96	0.40
1:C:670:ARG:NH1	1:C:704:ARG:HG2	2.37	0.40
1:E:433:ASP:HB3	1:E:541:ILE:HG12	2.02	0.40
1:F:795:PHE:O	1:F:797:ILE:N	2.55	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 PDB entries followed by that with respect to all EM entries.

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	642/972 (66%)	587 (91%)	54 (8%)	1 (0%)	43 71
1	B	642/972 (66%)	586 (91%)	53 (8%)	3 (0%)	24 55
1	C	642/972 (66%)	596 (93%)	45 (7%)	1 (0%)	43 71
1	D	640/972 (66%)	588 (92%)	49 (8%)	3 (0%)	24 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	864/972 (89%)	790 (91%)	71 (8%)	3 (0%)	36	64
1	F	642/972 (66%)	577 (90%)	62 (10%)	3 (0%)	24	55
All	All	4072/5832 (70%)	3724 (92%)	334 (8%)	14 (0%)	37	64

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	24	VAL
1	F	780	PHE
1	F	779	ARG
1	D	670	ARG
1	B	816	VAL
1	B	946	SER
1	C	946	SER
1	A	946	SER
1	E	291	SER
1	E	670	ARG
1	D	844	VAL
1	F	946	SER
1	B	297	ASP
1	D	946	SER

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 PDB entries followed by that with respect to all EM entries.

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	581/879 (66%)	563 (97%)	18 (3%)	35	61
1	B	581/879 (66%)	575 (99%)	6 (1%)	68	76
1	C	581/879 (66%)	571 (98%)	10 (2%)	53	70
1	D	579/879 (66%)	574 (99%)	5 (1%)	70	77
1	E	787/879 (90%)	781 (99%)	6 (1%)	73	78
1	F	581/879 (66%)	570 (98%)	11 (2%)	50	69
All	All	3690/5274 (70%)	3634 (98%)	56 (2%)	55	72

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	LYS
1	A	306	ILE
1	A	307	LEU
1	A	310	LEU
1	A	315	TYR
1	A	318	TYR
1	A	320	LEU
1	A	325	VAL
1	A	751	ARG
1	A	776	GLU
1	A	779	ARG
1	A	781	ILE
1	A	783	GLU
1	A	786	MET
1	A	789	ASP
1	A	791	GLN
1	A	868	THR
1	A	872	VAL
1	B	640	ASN
1	B	642	LYS
1	B	645	LEU
1	B	867	ASN
1	B	870	ILE
1	B	872	VAL
1	C	371	LYS
1	C	372	LYS
1	C	373	ILE
1	C	375	LYS
1	C	376	ARG
1	C	639	CYS
1	C	640	ASN
1	C	642	LYS
1	C	646	MET
1	C	870	ILE
1	D	642	LYS
1	D	645	LEU
1	D	646	MET
1	D	751	ARG
1	D	752	ARG
1	E	639	CYS
1	E	642	LYS
1	E	645	LEU

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Mol	Chain	Res	Type
1	E	752	ARG
1	E	870	ILE
1	E	871	ASN
1	F	639	CYS
1	F	642	LYS
1	F	645	LEU
1	F	646	MET
1	F	774	LYS
1	F	776	GLU
1	F	781	ILE
1	F	782	HIS
1	F	783	GLU
1	F	789	ASP
1	F	791	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	330	ASN
1	A	363	ASN
1	A	549	HIS
1	A	555	ASN
1	A	578	GLN
1	A	710	ASN
1	A	723	GLN
1	A	727	GLN
1	A	737	ASN
1	A	792	ASN
1	A	836	HIS
1	B	323	ASN
1	B	450	GLN
1	B	491	HIS
1	B	496	HIS
1	B	695	ASN
1	B	721	GLN
1	B	737	ASN
1	B	810	ASN
1	B	812	GLN
1	B	867	ASN
1	B	886	ASN
1	C	330	ASN

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Mol	Chain	Res	Type
1	C	368	HIS
1	C	470	HIS
1	C	487	HIS
1	C	491	HIS
1	C	577	HIS
1	C	721	GLN
1	C	764	HIS
1	C	792	ASN
1	C	867	ASN
1	C	875	HIS
1	C	948	ASN
1	D	389	GLN
1	D	496	HIS
1	D	710	ASN
1	D	747	HIS
1	D	782	HIS
1	D	812	GLN
1	D	882	GLN
1	E	71	HIS
1	E	105	ASN
1	E	308	ASN
1	E	330	ASN
1	E	363	ASN
1	E	415	HIS
1	E	491	HIS
1	E	677	ASN
1	E	747	HIS
1	E	764	HIS
1	E	765	ASN
1	E	792	ASN
1	E	806	GLN
1	E	871	ASN
1	E	875	HIS
1	F	323	ASN
1	F	491	HIS
1	F	555	ASN
1	F	640	ASN
1	F	695	ASN
1	F	701	ASN
1	F	782	HIS
1	F	871	ASN
1	F	916	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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$
4	ADP	F	1001	5	28,29,29	1.41	4 (14%)	43,45,45	1.83	10 (23%)
4	ADP	B	1001	5	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
4	ADP	C	1001	5	28,29,29	1.40	6 (21%)	43,45,45	1.90	12 (27%)
4	ADP	E	1001	5	28,29,29	1.37	6 (21%)	43,45,45	1.87	11 (25%)
4	ADP	D	1001	5	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
4	ADP	A	1001	5	28,29,29	1.39	4 (14%)	43,45,45	1.83	10 (23%)

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
4	ADP	F	1001	5	-	8/16/32/32	0/3/3/3
4	ADP	B	1001	5	-	8/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	C	1001	5	-	3/16/32/32	0/3/3/3
4	ADP	E	1001	5	-	8/16/32/32	0/3/3/3
4	ADP	D	1001	5	-	3/16/32/32	0/3/3/3
4	ADP	A	1001	5	-	5/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1001	ADP	C5-C4	4.73	1.47	1.39
4	B	1001	ADP	C5-C4	4.67	1.47	1.39
4	A	1001	ADP	C5-C4	4.64	1.47	1.39
4	D	1001	ADP	C5-C4	4.62	1.47	1.39
4	E	1001	ADP	C5-C4	4.12	1.46	1.39
4	C	1001	ADP	C5-C4	3.83	1.45	1.39
4	C	1001	ADP	C5-N7	-2.82	1.33	1.39
4	E	1001	ADP	C5-N7	-2.71	1.34	1.39
4	B	1001	ADP	C5-C6	2.68	1.48	1.41
4	F	1001	ADP	C5-C6	2.68	1.48	1.41
4	A	1001	ADP	C5-C6	2.67	1.48	1.41
4	C	1001	ADP	C4-N9	-2.64	1.32	1.37
4	D	1001	ADP	C5-C6	2.64	1.48	1.41
4	E	1001	ADP	C4-N9	-2.56	1.32	1.37
4	C	1001	ADP	C8-N9	-2.44	1.33	1.37
4	E	1001	ADP	C5-C6	2.36	1.47	1.41
4	A	1001	ADP	C8-N7	2.31	1.36	1.31
4	D	1001	ADP	C5-N7	-2.30	1.34	1.39
4	B	1001	ADP	C5-N7	-2.30	1.34	1.39
4	F	1001	ADP	C8-N7	2.28	1.36	1.31
4	B	1001	ADP	C8-N7	2.28	1.36	1.31
4	F	1001	ADP	C5-N7	-2.27	1.34	1.39
4	D	1001	ADP	C8-N7	2.25	1.36	1.31
4	A	1001	ADP	C5-N7	-2.25	1.35	1.39
4	C	1001	ADP	C5-C6	2.24	1.47	1.41
4	E	1001	ADP	C8-N9	-2.09	1.34	1.37
4	C	1001	ADP	C8-N7	2.03	1.35	1.31
4	E	1001	ADP	C8-N7	2.01	1.35	1.31

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1001	ADP	C5-C4-N3	-5.76	118.79	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	ADP	C5-C4-N3	-5.73	118.82	126.72
4	F	1001	ADP	C5-C4-N3	-5.72	118.85	126.72
4	A	1001	ADP	C5-C4-N3	-5.64	118.96	126.72
4	C	1001	ADP	C5-C4-N3	-5.56	119.07	126.72
4	E	1001	ADP	C5-C4-N3	-5.44	119.23	126.72
4	D	1001	ADP	N3-C4-N9	4.66	135.10	127.17
4	F	1001	ADP	N3-C4-N9	4.61	135.01	127.17
4	B	1001	ADP	N3-C4-N9	4.56	134.92	127.17
4	A	1001	ADP	N3-C4-N9	4.55	134.91	127.17
4	C	1001	ADP	N3-C4-N9	4.46	134.76	127.17
4	E	1001	ADP	N3-C4-N9	4.40	134.65	127.17
4	D	1001	ADP	C2-N3-C4	3.63	120.70	111.83
4	B	1001	ADP	C2-N3-C4	3.63	120.69	111.83
4	A	1001	ADP	C2-N3-C4	3.62	120.67	111.83
4	F	1001	ADP	C2-N3-C4	3.60	120.62	111.83
4	C	1001	ADP	C2-N3-C4	3.60	120.61	111.83
4	C	1001	ADP	C4-C5-N7	-3.58	106.49	110.58
4	E	1001	ADP	C2-N3-C4	3.50	120.39	111.83
4	E	1001	ADP	C4-C5-N7	-3.47	106.61	110.58
4	C	1001	ADP	C4-N9-C8	3.45	109.36	105.74
4	B	1001	ADP	C4-C5-N7	-3.41	106.68	110.58
4	A	1001	ADP	C4-C5-N7	-3.40	106.70	110.58
4	F	1001	ADP	C4-C5-N7	-3.38	106.72	110.58
4	D	1001	ADP	C4-C5-N7	-3.36	106.74	110.58
4	E	1001	ADP	C4-N9-C8	3.27	109.17	105.74
4	C	1001	ADP	N3-C2-N1	-3.25	123.67	128.58
4	A	1001	ADP	N3-C2-N1	-3.21	123.73	128.58
4	D	1001	ADP	N3-C2-N1	-3.19	123.75	128.58
4	E	1001	ADP	N3-C2-N1	-3.17	123.78	128.58
4	B	1001	ADP	N3-C2-N1	-3.15	123.82	128.58
4	F	1001	ADP	N3-C2-N1	-3.14	123.83	128.58
4	A	1001	ADP	C4-N9-C8	2.93	108.81	105.74
4	D	1001	ADP	C4-N9-C8	2.83	108.71	105.74
4	F	1001	ADP	C4-N9-C8	2.80	108.68	105.74
4	C	1001	ADP	C5-N7-C8	2.66	107.64	103.45
4	B	1001	ADP	C4-N9-C8	2.66	108.53	105.74
4	E	1001	ADP	C2'-C1'-N9	-2.64	106.74	113.30
4	E	1001	ADP	C5-N7-C8	2.58	107.50	103.45
4	D	1001	ADP	C5-N7-C8	2.53	107.43	103.45
4	C	1001	ADP	N9-C8-N7	-2.53	110.34	113.94
4	F	1001	ADP	C5-N7-C8	2.51	107.39	103.45
4	A	1001	ADP	C5-N7-C8	2.50	107.38	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	ADP	C5-N7-C8	2.50	107.37	103.45
4	D	1001	ADP	C3'-C2'-C1'	2.46	106.12	101.46
4	A	1001	ADP	C3'-C2'-C1'	2.43	106.05	101.46
4	F	1001	ADP	C3'-C2'-C1'	2.39	105.99	101.46
4	E	1001	ADP	N9-C8-N7	-2.36	110.59	113.94
4	C	1001	ADP	C3'-C2'-C1'	2.20	105.63	101.46
4	B	1001	ADP	C3'-C2'-C1'	2.19	105.61	101.46
4	C	1001	ADP	C6-C5-N7	2.18	136.30	132.09
4	E	1001	ADP	C3'-C2'-C1'	2.17	105.57	101.46
4	A	1001	ADP	C6-C5-N7	2.13	136.19	132.09
4	E	1001	ADP	C6-C5-N7	2.09	136.12	132.09
4	A	1001	ADP	N9-C8-N7	-2.08	110.98	113.94
4	C	1001	ADP	C2'-C3'-C4'	2.08	106.63	102.61
4	B	1001	ADP	C6-C5-N7	2.08	136.10	132.09
4	D	1001	ADP	N9-C8-N7	-2.07	111.00	113.94
4	C	1001	ADP	O3B-PB-O2B	2.03	115.40	107.80
4	F	1001	ADP	C6-C5-N7	2.02	135.98	132.09
4	F	1001	ADP	N9-C8-N7	-2.02	111.08	113.94

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	ADP	PA-O3A-PB-O2B
4	A	1001	ADP	C5'-O5'-PA-O3A
4	B	1001	ADP	PA-O3A-PB-O3B
4	B	1001	ADP	C5'-O5'-PA-O3A
4	B	1001	ADP	C4'-C5'-O5'-PA
4	C	1001	ADP	C5'-O5'-PA-O3A
4	D	1001	ADP	C5'-O5'-PA-O2A
4	D	1001	ADP	C5'-O5'-PA-O3A
4	D	1001	ADP	C4'-C5'-O5'-PA
4	E	1001	ADP	PB-O3A-PA-O5'
4	E	1001	ADP	C5'-O5'-PA-O1A
4	E	1001	ADP	C5'-O5'-PA-O2A
4	E	1001	ADP	C5'-O5'-PA-O3A
4	F	1001	ADP	PA-O3A-PB-O2B
4	F	1001	ADP	PA-O3A-PB-O3B
4	F	1001	ADP	C3'-C4'-C5'-O5'
4	B	1001	ADP	O4'-C4'-C5'-O5'
4	B	1001	ADP	C3'-C4'-C5'-O5'
4	F	1001	ADP	O4'-C4'-C5'-O5'

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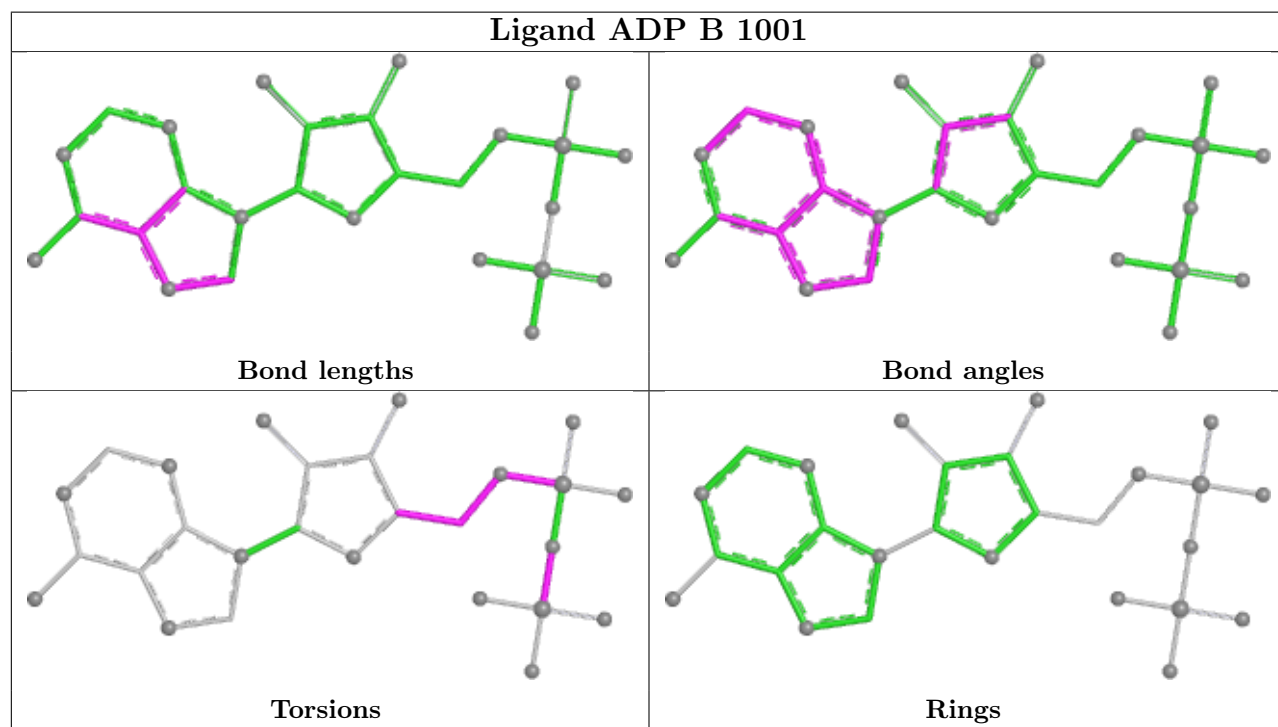
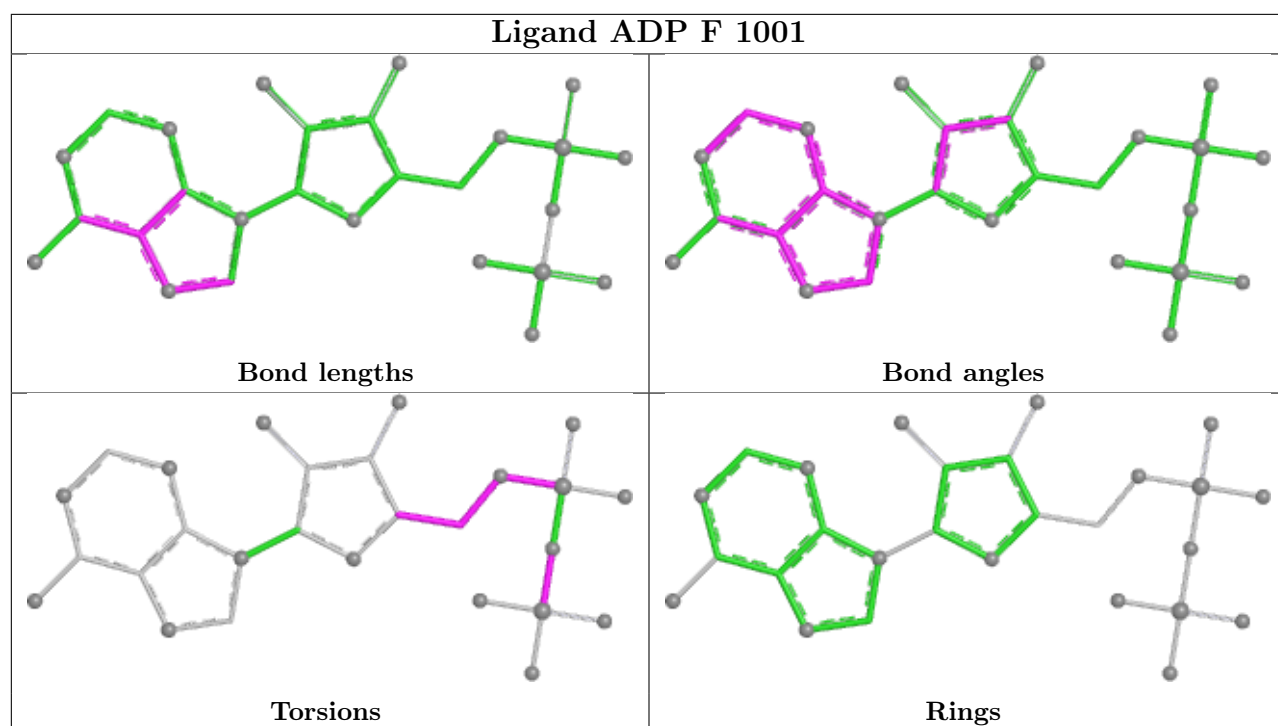
Mol	Chain	Res	Type	Atoms
4	C	1001	ADP	O4'-C4'-C5'-O5'
4	C	1001	ADP	C3'-C4'-C5'-O5'
4	E	1001	ADP	PA-O3A-PB-O1B
4	E	1001	ADP	PA-O3A-PB-O3B
4	A	1001	ADP	C5'-O5'-PA-O1A
4	B	1001	ADP	C5'-O5'-PA-O1A
4	F	1001	ADP	C5'-O5'-PA-O1A
4	F	1001	ADP	C5'-O5'-PA-O2A
4	F	1001	ADP	C5'-O5'-PA-O3A
4	E	1001	ADP	C4'-C5'-O5'-PA
4	F	1001	ADP	C4'-C5'-O5'-PA
4	E	1001	ADP	O4'-C4'-C5'-O5'
4	B	1001	ADP	PA-O3A-PB-O1B
4	A	1001	ADP	PA-O3A-PB-O3B
4	B	1001	ADP	PA-O3A-PB-O2B
4	A	1001	ADP	PA-O3A-PB-O1B

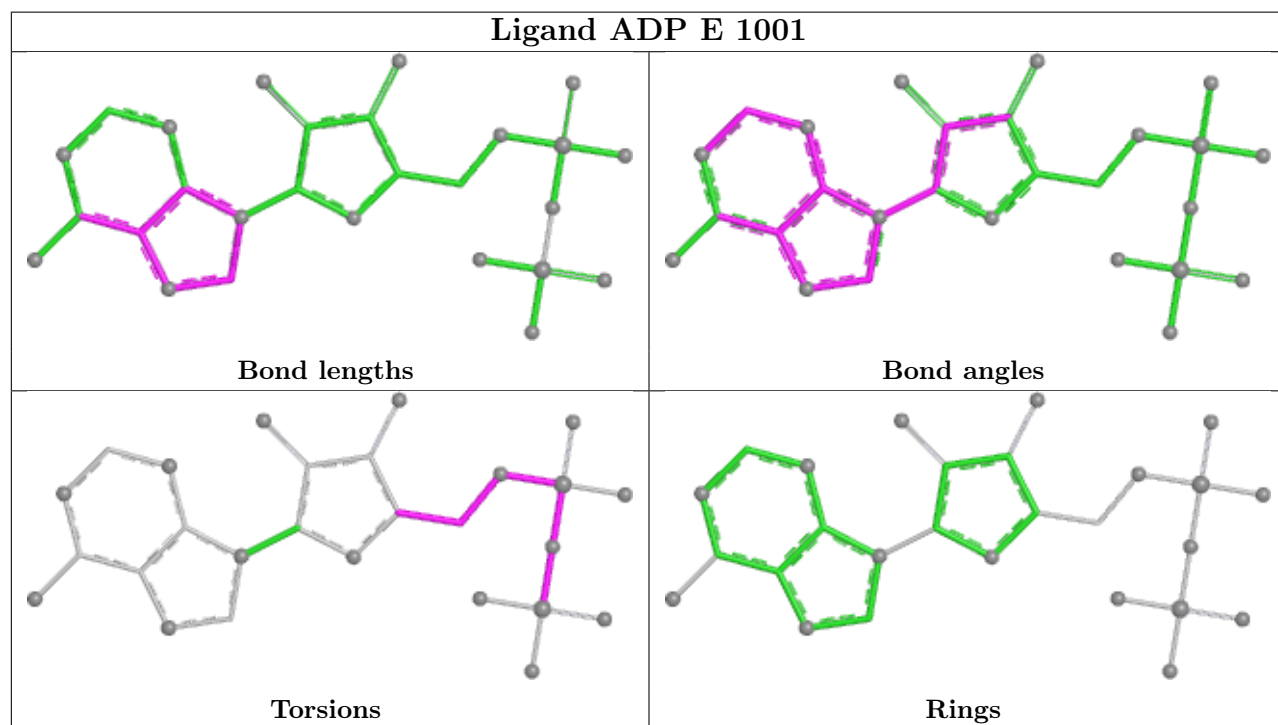
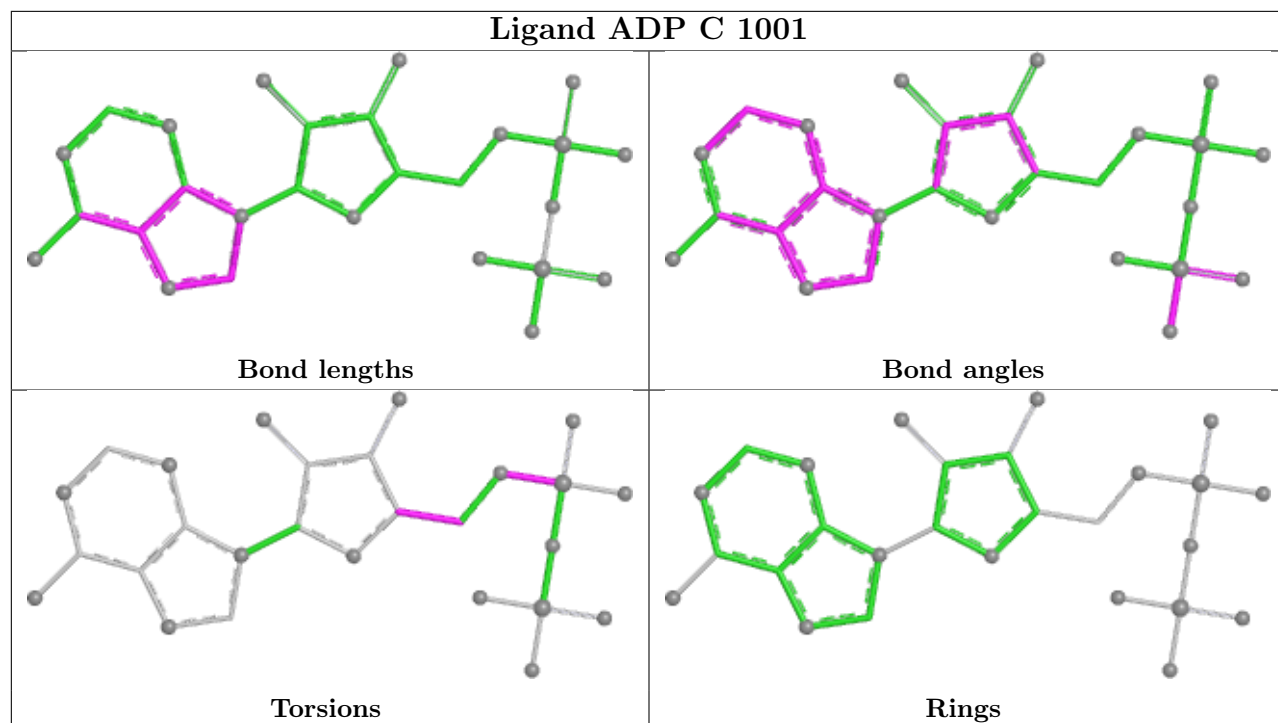
There are no ring outliers.

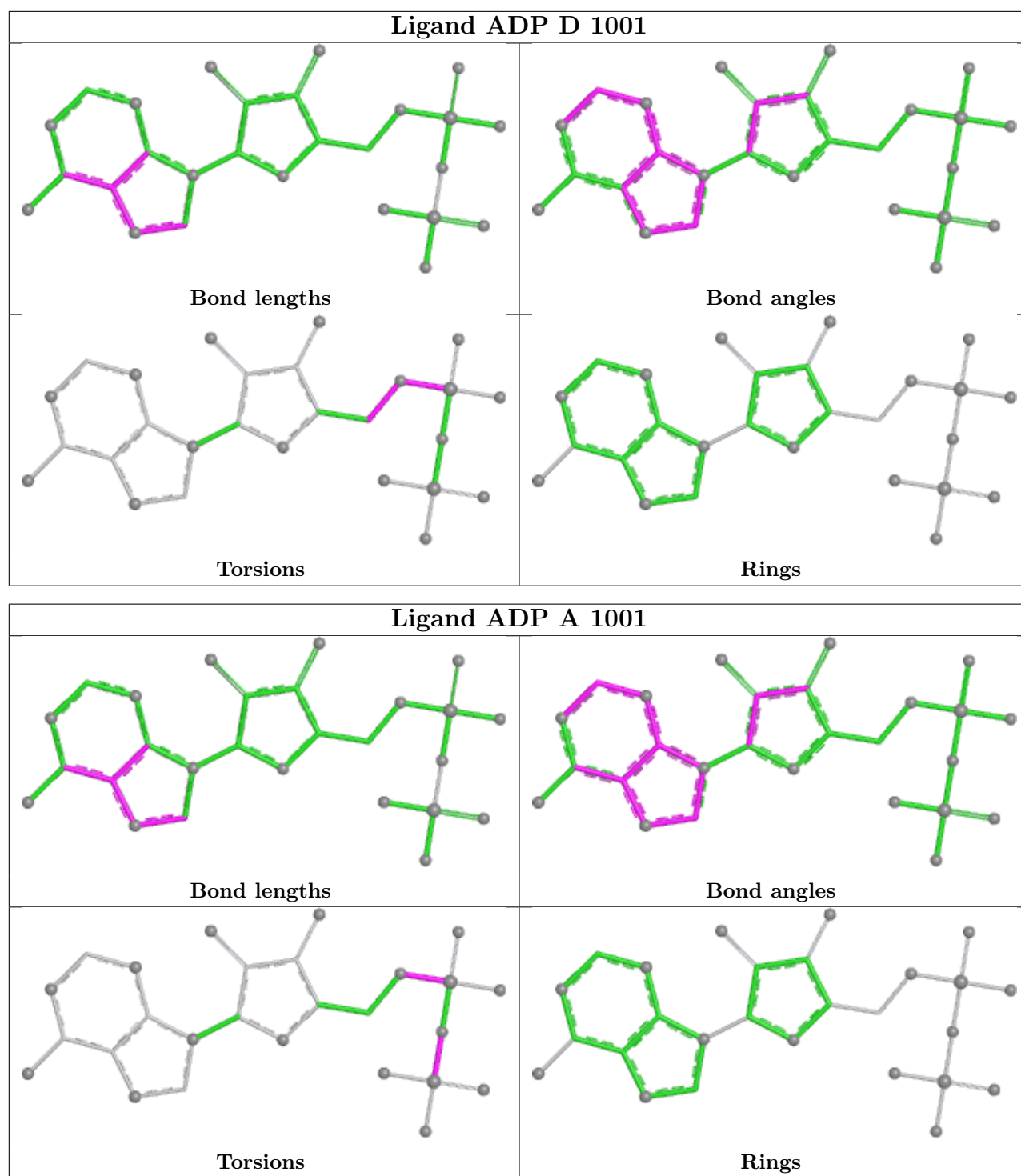
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1001	ADP	2	0
4	B	1001	ADP	2	0
4	C	1001	ADP	2	0
4	E	1001	ADP	2	0
4	D	1001	ADP	4	0
4	A	1001	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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 Map visualisation

This section contains visualisations of the EMDB entry EMD-37880. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.