



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:12 PM UTC

PDB ID : 1MX0 / pdb_00001mx0
Title : Structure of topoisomerase subunit
Authors : Corbett, K.D.; Berger, J.M.
Deposited on : 2002-10-01
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

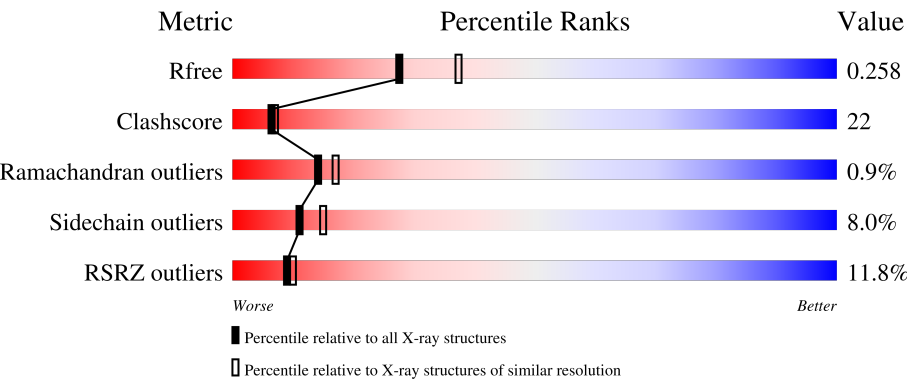
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	472	5% 62%33%..
1	B	472	2% 66%28%..
1	C	472	2% 68%28%..
1	D	472	2% 71%22%..
1	E	472	3% 63%29%5%.

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Mol	Chain	Length	Quality of chain
1	F	472	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23057 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 Type II DNA topoisomerase VI subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	Se	0	0	0
			3704	2384	620	694	1	5			
1	B	455	Total	C	N	O	S	Se	0	0	0
			3651	2352	608	685	1	5			
1	C	466	Total	C	N	O	S	Se	0	0	0
			3738	2404	626	702	1	5			
1	D	461	Total	C	N	O	S	Se	0	0	0
			3687	2374	615	692	1	5			
1	E	456	Total	C	N	O	S	Se	0	0	0
			3677	2368	614	689	1	5			
1	F	454	Total	C	N	O	S	Se	0	0	0
			3596	2316	598	676	1	5			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O05207
A	0	ALA	-	expression tag	UNP O05207
A	107	MSE	MET	modified residue	UNP O05207
A	121	MSE	MET	modified residue	UNP O05207
A	303	TYR	ASP	SEE REMARK 999	UNP O05207
A	409	MSE	MET	modified residue	UNP O05207
A	412	MSE	MET	modified residue	UNP O05207
A	435	ASP	ASN	SEE REMARK 999	UNP O05207
A	445	MSE	MET	modified residue	UNP O05207
B	-1	GLY	-	expression tag	UNP O05207
B	0	ALA	-	expression tag	UNP O05207
B	107	MSE	MET	modified residue	UNP O05207
B	121	MSE	MET	modified residue	UNP O05207
B	303	TYR	ASP	SEE REMARK 999	UNP O05207
B	409	MSE	MET	modified residue	UNP O05207
B	412	MSE	MET	modified residue	UNP O05207
B	435	ASP	ASN	SEE REMARK 999	UNP O05207

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Chain	Residue	Modelled	Actual	Comment	Reference
B	445	MSE	MET	modified residue	UNP O05207
C	-1	GLY	-	expression tag	UNP O05207
C	0	ALA	-	expression tag	UNP O05207
C	107	MSE	MET	modified residue	UNP O05207
C	121	MSE	MET	modified residue	UNP O05207
C	303	TYR	ASP	SEE REMARK 999	UNP O05207
C	409	MSE	MET	modified residue	UNP O05207
C	412	MSE	MET	modified residue	UNP O05207
C	435	ASP	ASN	SEE REMARK 999	UNP O05207
C	445	MSE	MET	modified residue	UNP O05207
D	-1	GLY	-	expression tag	UNP O05207
D	0	ALA	-	expression tag	UNP O05207
D	107	MSE	MET	modified residue	UNP O05207
D	121	MSE	MET	modified residue	UNP O05207
D	303	TYR	ASP	SEE REMARK 999	UNP O05207
D	409	MSE	MET	modified residue	UNP O05207
D	412	MSE	MET	modified residue	UNP O05207
D	435	ASP	ASN	SEE REMARK 999	UNP O05207
D	445	MSE	MET	modified residue	UNP O05207
E	-1	GLY	-	expression tag	UNP O05207
E	0	ALA	-	expression tag	UNP O05207
E	107	MSE	MET	modified residue	UNP O05207
E	121	MSE	MET	modified residue	UNP O05207
E	303	TYR	ASP	SEE REMARK 999	UNP O05207
E	409	MSE	MET	modified residue	UNP O05207
E	412	MSE	MET	modified residue	UNP O05207
E	435	ASP	ASN	SEE REMARK 999	UNP O05207
E	445	MSE	MET	modified residue	UNP O05207
F	-1	GLY	-	expression tag	UNP O05207
F	0	ALA	-	expression tag	UNP O05207
F	107	MSE	MET	modified residue	UNP O05207
F	121	MSE	MET	modified residue	UNP O05207
F	303	TYR	ASP	SEE REMARK 999	UNP O05207
F	409	MSE	MET	modified residue	UNP O05207
F	412	MSE	MET	modified residue	UNP O05207
F	435	ASP	ASN	SEE REMARK 999	UNP O05207
F	445	MSE	MET	modified residue	UNP O05207

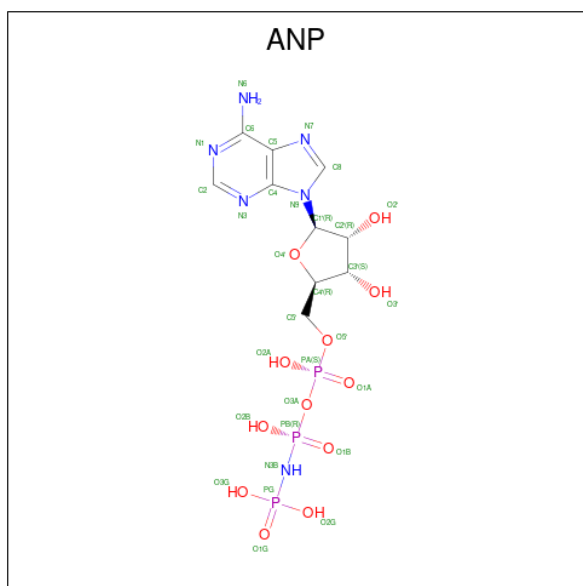
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 10 6 12 3	0	0
3	B	1	Total C N O P 31 10 6 12 3	0	0
3	C	1	Total C N O P 31 10 6 12 3	0	0
3	D	1	Total C N O P 31 10 6 12 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

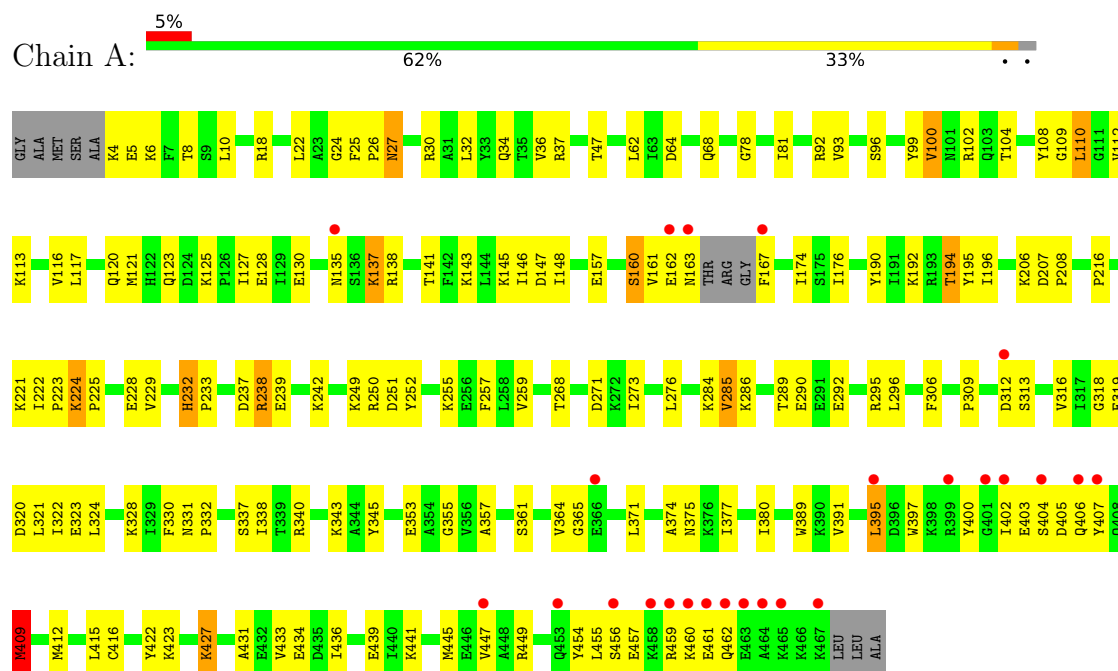
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total	O	0	0
			160	160		
5	B	145	Total	O	0	0
			145	145		
5	C	140	Total	O	0	0
			140	140		
5	D	160	Total	O	0	0
			160	160		
5	E	125	Total	O	0	0
			125	125		
5	F	81	Total	O	0	0
			81	81		

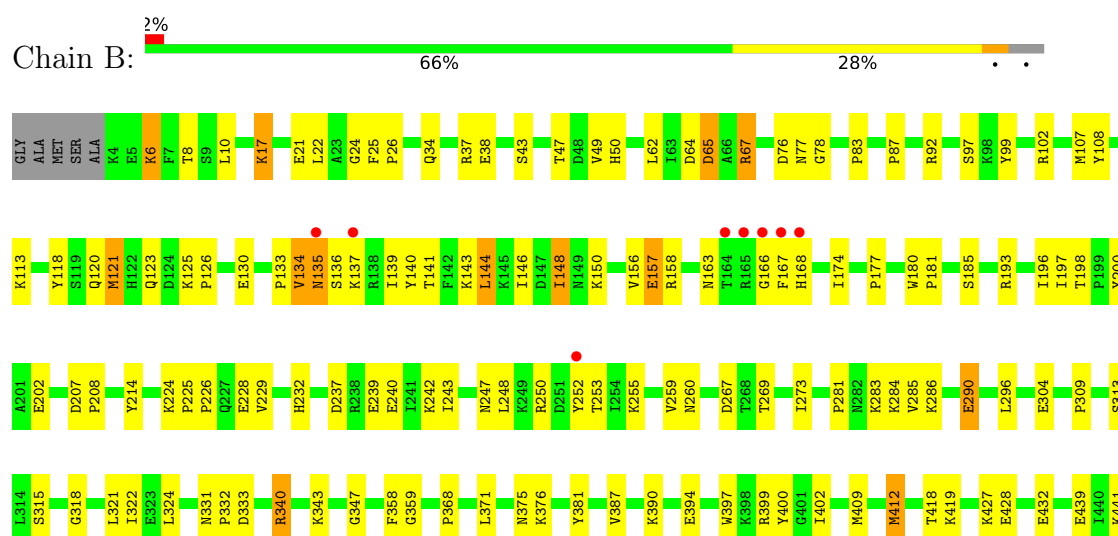
3 Residue-property plots

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

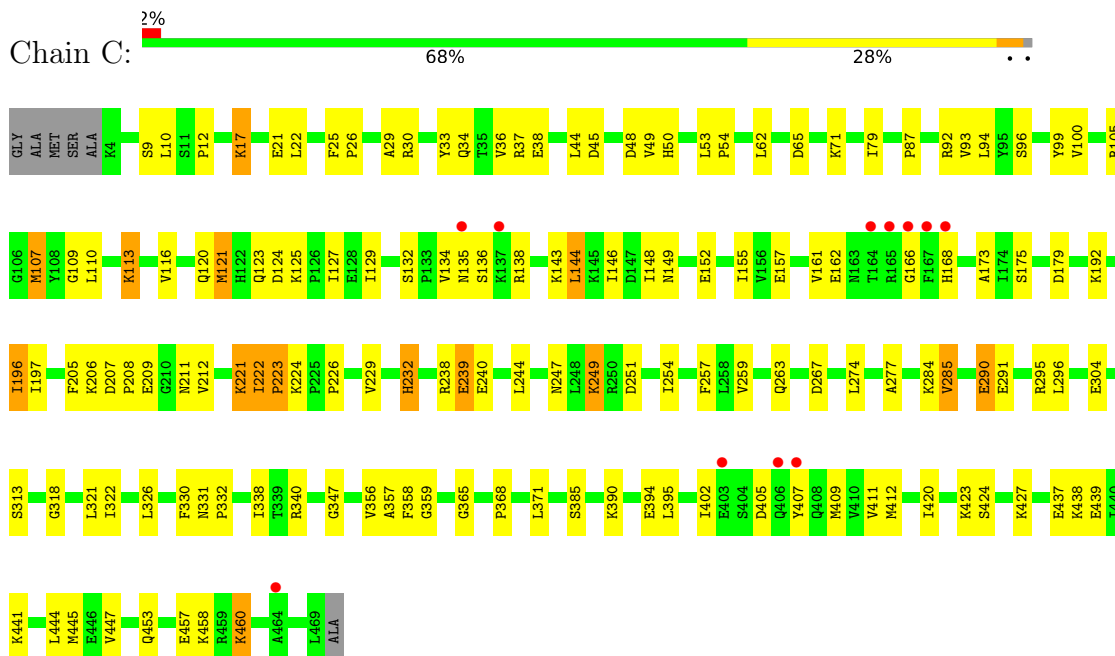
• Molecule 1: Type II DNA topoisomerase VI subunit B



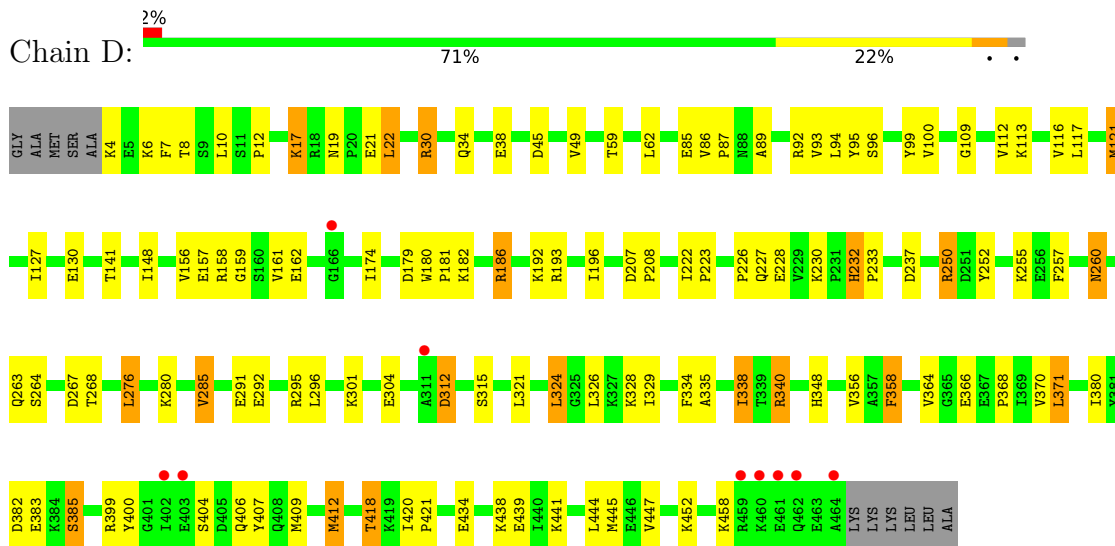
• Molecule 1: Type II DNA topoisomerase VI subunit B



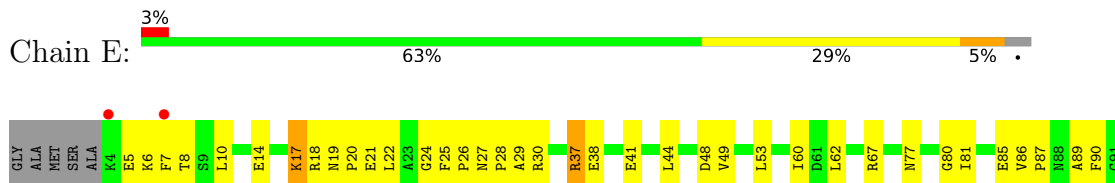
- Molecule 1: Type II DNA topoisomerase VI subunit B

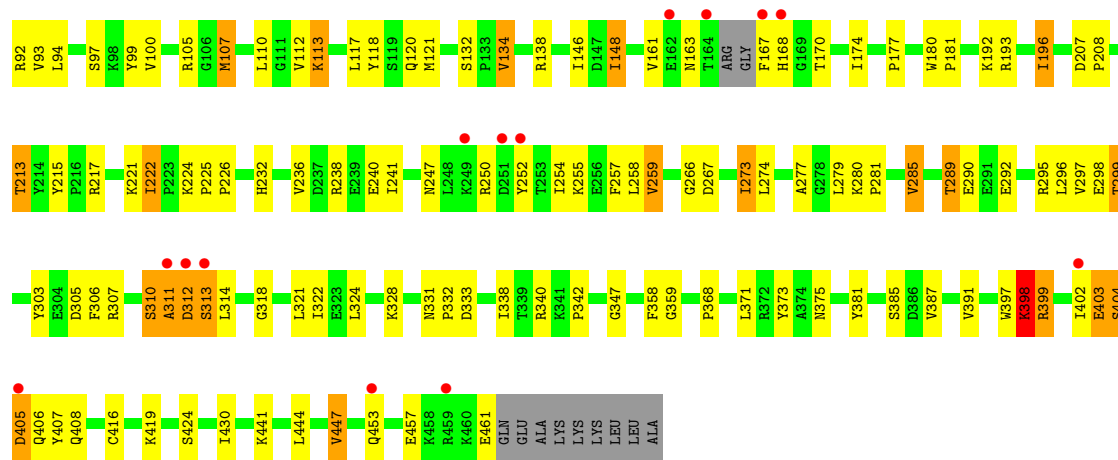


- Molecule 1: Type II DNA topoisomerase VI subunit B

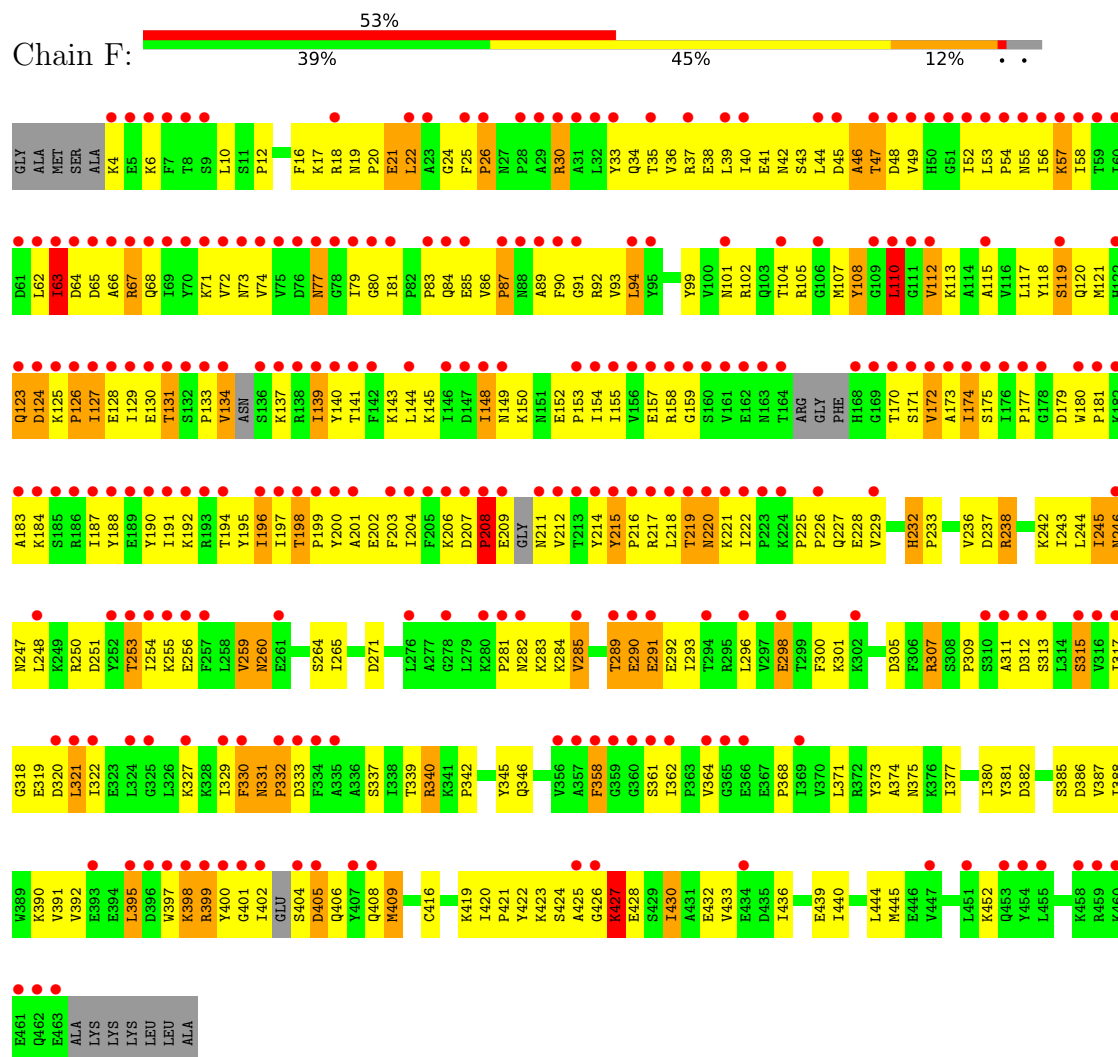


- Molecule 1: Type II DNA topoisomerase VI subunit B





● Molecule 1: Type II DNA topoisomerase VI subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.66Å 219.19Å 106.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.30) 97.9 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.214 , 0.263 0.216 , 0.258	Depositor DCC
R_{free} test set	12540 reflections (8.36%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23057	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.78	0/3779	1.01	6/5104 (0.1%)
1	B	0.81	2/3727 (0.1%)	1.02	3/5038 (0.1%)
1	C	0.76	2/3814 (0.1%)	0.99	9/5152 (0.2%)
1	D	0.78	2/3763 (0.1%)	1.00	4/5087 (0.1%)
1	E	0.76	1/3752 (0.0%)	0.99	10/5067 (0.2%)
1	F	0.59	0/3666	1.06	22/4955 (0.4%)
All	All	0.75	7/22501 (0.0%)	1.01	54/30403 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	MSE	SE-CE	-9.74	1.66	1.95
1	C	107	MSE	SE-CE	7.12	2.16	1.95
1	D	121	MSE	SE-CE	-6.80	1.75	1.95
1	E	107	MSE	SE-CE	-6.54	1.75	1.95
1	D	412	MSE	SE-CE	5.72	2.12	1.95
1	B	121	MSE	SE-CE	-5.53	1.78	1.95
1	C	121	MSE	SE-CE	-5.49	1.78	1.95

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	330	PHE	N-CA-C	-10.95	92.92	110.32
1	F	427	LYS	N-CA-C	10.10	123.64	111.02
1	F	108	TYR	N-CA-C	9.37	124.84	113.41
1	D	358	PHE	N-CA-C	9.26	123.30	110.06
1	F	110	LEU	N-CA-C	7.86	122.24	111.71
1	C	405	ASP	N-CA-C	-7.86	103.69	113.28
1	D	232	HIS	N-CA-C	-7.85	100.19	110.39
1	C	232	HIS	N-CA-C	-7.39	100.11	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	333	ASP	N-CA-C	-7.36	104.16	113.43
1	F	137	LYS	N-CA-C	-7.27	104.40	113.20
1	B	418	THR	N-CA-C	-7.07	104.62	113.18
1	A	457	GLU	N-CA-C	-6.68	105.28	113.50
1	F	232	HIS	N-CA-C	-6.54	101.83	110.07
1	D	260	ASN	N-CA-C	6.49	118.43	111.36
1	F	67	ARG	N-CA-C	-6.11	104.94	113.37
1	F	123	GLN	N-CA-C	6.02	116.37	107.88
1	C	223	PRO	CA-C-O	-6.00	114.97	121.27
1	F	215	TYR	CA-C-N	5.96	127.29	119.84
1	F	215	TYR	C-N-CA	5.96	127.29	119.84
1	F	260	ASN	N-CA-C	5.96	120.73	112.45
1	E	311	ALA	N-CA-C	-5.80	106.29	113.19
1	A	409	MSE	N-CA-C	5.76	118.88	108.69
1	C	222	ILE	CA-C-N	5.74	126.64	119.98
1	C	222	ILE	C-N-CA	5.74	126.64	119.98
1	C	223	PRO	N-CA-C	5.63	120.08	110.95
1	E	399	ARG	N-CA-C	-5.58	106.31	114.39
1	F	409	MSE	N-CA-C	5.57	118.27	108.75
1	F	427	LYS	CA-C-N	-5.48	112.47	122.38
1	F	427	LYS	C-N-CA	-5.48	112.47	122.38
1	F	358	PHE	CA-C-N	-5.47	116.23	122.42
1	F	358	PHE	C-N-CA	-5.47	116.23	122.42
1	E	314	LEU	N-CA-C	-5.41	101.14	109.52
1	F	321	LEU	N-CA-C	-5.38	107.09	113.97
1	E	405	ASP	N-CA-C	-5.35	106.81	113.55
1	E	148	ILE	N-CA-C	5.34	115.55	110.42
1	F	358	PHE	N-CA-C	5.33	122.12	114.39
1	C	36	VAL	CA-C-N	5.29	127.31	120.44
1	C	36	VAL	C-N-CA	5.29	127.31	120.44
1	A	232	HIS	N-CA-C	-5.27	103.43	110.07
1	F	108	TYR	CB-CA-C	-5.23	100.09	109.24
1	E	403	GLU	CB-CA-C	5.22	120.81	110.42
1	F	305	ASP	N-CA-C	5.21	119.21	111.87
1	E	97	SER	N-CA-C	-5.20	106.17	112.88
1	A	377	ILE	CB-CA-C	-5.20	104.81	110.37
1	F	427	LYS	CB-CA-C	-5.15	102.83	112.30
1	D	156	VAL	CB-CA-C	-5.14	105.19	112.14
1	B	37	ARG	CB-CA-C	-5.14	102.81	110.88
1	A	36	VAL	CA-C-N	5.11	127.09	120.44
1	A	36	VAL	C-N-CA	5.11	127.09	120.44
1	E	333	ASP	N-CA-C	-5.09	106.24	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	GLU	N-CA-C	-5.08	107.08	113.28
1	B	135	ASN	N-CA-C	5.07	121.59	110.80
1	E	408	GLN	N-CA-C	-5.06	102.61	109.54
1	E	313	SER	N-CA-C	5.05	121.55	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3704	0	3760	160	0
1	B	3651	0	3704	124	0
1	C	3738	0	3792	140	0
1	D	3687	0	3735	104	0
1	E	3677	0	3746	142	0
1	F	3596	0	3605	341	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	2	0
3	C	31	0	13	0	0
3	D	31	0	13	1	0
3	E	31	0	13	1	0
3	F	31	0	13	4	0
4	D	1	0	0	0	0
5	A	160	0	0	21	0
5	B	145	0	0	19	0
5	C	140	0	0	18	0
5	D	160	0	0	23	0
5	E	125	0	0	19	0
5	F	81	0	0	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23057	0	22420	977	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 22.

All (977) 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:C:107:MSE:SE	1:C:107:MSE:CE	2.16	1.43
1:C:127:ILE:HD11	1:C:144:LEU:CD1	1.56	1.34
1:A:4:LYS:HD2	1:A:4:LYS:O	1.16	1.33
1:C:127:ILE:CD1	1:C:144:LEU:HD11	1.64	1.27
1:E:402:ILE:HG22	1:E:403:GLU:O	1.30	1.25
1:D:358:PHE:CD2	1:D:358:PHE:O	2.02	1.12
1:F:180:TRP:CG	1:F:208:PRO:HG2	1.84	1.12
1:F:203:PHE:HB2	1:F:215:TYR:HB2	1.31	1.10
1:F:53:LEU:HD23	1:F:222:ILE:HD11	1.25	1.10
1:C:238:ARG:HH22	1:C:290:GLU:HG3	1.04	1.07
1:A:4:LYS:HG2	5:B:962:HOH:O	1.53	1.06
1:A:239:GLU:HG3	5:A:1044:HOH:O	1.54	1.06
1:F:119:SER:O	1:F:123:GLN:HG3	1.56	1.05
1:F:117:LEU:HD22	1:F:148:ILE:HD13	1.36	1.04
1:B:441:LYS:HE2	1:B:445:MSE:HE3	1.10	1.04
1:F:53:LEU:CD2	1:F:222:ILE:HD11	1.87	1.04
1:C:322:ILE:HG23	1:C:412:MSE:HE3	1.39	1.03
1:D:250:ARG:CG	1:D:250:ARG:HH11	1.69	1.02
1:C:238:ARG:NH2	1:C:290:GLU:HG3	1.73	1.02
1:E:192:LYS:HG3	5:E:1044:HOH:O	1.58	1.02
1:E:120:GLN:NE2	1:E:146:ILE:H	1.58	1.01
1:F:198:THR:HG23	1:F:198:THR:O	1.56	1.01
1:A:313:SER:HA	5:A:1031:HOH:O	1.59	1.00
1:F:364:VAL:HG22	1:F:408:GLN:OE1	1.63	0.98
1:A:4:LYS:O	1:A:4:LYS:CD	2.11	0.98
1:E:120:GLN:HE22	1:E:146:ILE:N	1.60	0.97
1:A:409:MSE:SE	5:A:1021:HOH:O	2.31	0.96
1:E:37:ARG:HH11	1:E:37:ARG:CG	1.79	0.96
1:A:120:GLN:HE22	1:A:146:ILE:H	1.14	0.96
1:A:403:GLU:HG2	1:A:404:SER:H	1.30	0.95
1:F:143:LYS:HG3	1:F:157:GLU:HB3	1.45	0.95
1:B:120:GLN:NE2	1:B:146:ILE:H	1.66	0.94
1:C:322:ILE:HG23	1:C:412:MSE:CE	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:ASP:HB3	5:E:1047:HOH:O	1.66	0.94
1:B:120:GLN:HE22	1:B:146:ILE:N	1.66	0.93
1:D:358:PHE:O	1:D:358:PHE:CG	2.21	0.93
1:F:180:TRP:CD2	1:F:208:PRO:HG2	2.04	0.93
1:A:4:LYS:HD2	1:A:4:LYS:C	1.94	0.93
1:A:37:ARG:HH22	1:A:427:LYS:HB2	1.33	0.92
1:B:121:MSE:HE2	5:B:941:HOH:O	1.70	0.92
1:B:441:LYS:HE2	1:B:445:MSE:CE	1.98	0.92
1:B:441:LYS:CE	1:B:445:MSE:HE3	1.98	0.91
1:F:253:THR:CG2	1:F:256:GLU:HG3	2.01	0.91
1:C:120:GLN:HE22	1:C:146:ILE:H	1.13	0.91
1:C:453:GLN:HE21	1:C:457:GLU:HG3	1.32	0.91
1:F:53:LEU:HD23	1:F:222:ILE:CD1	2.00	0.90
1:C:134:VAL:HG23	5:C:1000:HOH:O	1.72	0.90
1:D:250:ARG:HH11	1:D:250:ARG:HG2	1.35	0.90
1:F:330:PHE:C	1:F:332:PRO:HD3	1.97	0.89
1:B:139:ILE:HG13	1:B:163:ASN:HB3	1.53	0.89
1:F:92:ARG:O	1:F:113:LYS:HE2	1.71	0.89
1:F:141:THR:OG1	1:F:159:GLY:HA3	1.72	0.89
1:A:137:LYS:CD	1:A:137:LYS:H	1.83	0.89
1:E:213:THR:HG22	1:E:215:TYR:CE2	2.08	0.88
1:F:83:PRO:HG3	1:F:140:TYR:CE2	2.07	0.88
1:F:154:ILE:HG12	5:F:978:HOH:O	1.72	0.88
1:F:55:ASN:H	1:F:77:ASN:HD21	1.22	0.88
1:C:135:ASN:HB2	5:C:969:HOH:O	1.71	0.87
1:E:163:ASN:HD21	1:E:167:PHE:HB3	1.38	0.87
1:A:37:ARG:NH2	1:A:427:LYS:HB2	1.90	0.87
1:A:316:VAL:HG13	1:A:353:GLU:CD	2.00	0.87
1:C:453:GLN:NE2	1:C:457:GLU:HG3	1.89	0.87
1:F:124:ASP:O	1:F:126:PRO:HD3	1.75	0.86
1:A:163:ASN:HB2	5:A:1024:HOH:O	1.75	0.86
1:B:136:SER:HB2	5:B:1008:HOH:O	1.74	0.86
1:B:340:ARG:HD3	1:B:439:GLU:OE2	1.76	0.86
1:E:213:THR:HG21	1:E:215:TYR:OH	1.75	0.86
1:A:229:VAL:HG11	1:A:313:SER:HB3	1.58	0.86
1:F:207:ASP:OD2	1:F:211:ASN:CB	2.23	0.86
1:F:198:THR:O	1:F:198:THR:CG2	2.22	0.85
1:A:138:ARG:HH21	1:A:160:SER:HB3	1.40	0.85
1:E:311:ALA:HB2	1:E:342:PRO:CG	2.07	0.85
1:A:397:TRP:CD2	1:A:409:MSE:HE1	2.12	0.84
1:B:130:GLU:HG2	1:B:141:THR:HG22	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:LYS:HD2	5:C:1008:HOH:O	1.76	0.84
1:F:127:ILE:HD12	1:F:174:ILE:HD13	1.58	0.84
1:F:229:VAL:HG11	1:F:313:SER:HB3	1.59	0.84
1:E:213:THR:CG2	1:E:215:TYR:CZ	2.60	0.84
1:D:179:ASP:OD2	1:D:182:LYS:HD2	1.78	0.83
1:F:381:TYR:HB2	1:F:428:GLU:HG3	1.60	0.83
1:C:17:LYS:NZ	1:C:121:MSE:HE3	1.93	0.83
1:F:206:LYS:HG3	1:F:211:ASN:O	1.77	0.83
1:C:277:ALA:O	1:C:295:ARG:HD2	1.76	0.83
1:A:137:LYS:H	1:A:137:LYS:HD2	1.44	0.83
1:F:155:ILE:HG22	5:F:1013:HOH:O	1.80	0.82
1:A:123:GLN:NE2	1:A:125:LYS:H	1.77	0.82
1:E:295:ARG:CZ	5:E:1054:HOH:O	2.26	0.82
1:C:424:SER:HB2	5:C:1057:HOH:O	1.80	0.81
1:A:316:VAL:HG13	1:A:353:GLU:OE2	1.80	0.81
1:F:245:ILE:HG22	1:F:246:ASN:N	1.95	0.81
1:B:250:ARG:HH11	1:B:252:TYR:HE1	1.29	0.81
1:E:257:PHE:HB2	1:E:285:VAL:HG21	1.63	0.81
1:F:311:ALA:HB2	1:F:342:PRO:CG	2.10	0.81
1:E:295:ARG:O	1:E:299:THR:HG22	1.81	0.81
1:B:239:GLU:O	1:B:243:ILE:HD13	1.80	0.80
1:B:322:ILE:HG23	1:B:412:MSE:HE3	1.64	0.80
1:F:183:ALA:O	1:F:187:ILE:HG13	1.82	0.80
1:B:445:MSE:HE2	5:B:1048:HOH:O	1.80	0.79
1:C:322:ILE:CG2	1:C:412:MSE:HE3	2.11	0.79
1:E:132:SER:O	1:E:168:HIS:HA	1.81	0.79
1:F:206:LYS:HA	1:F:211:ASN:O	1.82	0.79
1:E:311:ALA:HB2	1:E:342:PRO:HG2	1.63	0.79
1:E:37:ARG:HH11	1:E:37:ARG:HG3	1.47	0.79
1:F:327:LYS:HA	1:F:332:PRO:HD2	1.62	0.79
1:C:249:LYS:HE2	1:C:249:LYS:HA	1.63	0.79
1:D:250:ARG:HH11	1:D:250:ARG:HG3	1.44	0.78
1:C:120:GLN:HE22	1:C:146:ILE:N	1.80	0.78
1:A:331:ASN:N	1:A:332:PRO:HD3	1.98	0.78
1:C:127:ILE:CD1	1:C:144:LEU:CD1	2.39	0.78
1:F:253:THR:HG23	1:F:256:GLU:HB2	1.65	0.78
3:F:950:ANP:H2'	5:F:951:HOH:O	1.83	0.78
1:A:130:GLU:HG2	1:A:141:THR:HG22	1.65	0.78
1:F:117:LEU:HD22	1:F:148:ILE:CD1	2.12	0.78
1:F:207:ASP:OD2	1:F:211:ASN:HB3	1.84	0.77
1:E:213:THR:HG22	1:E:215:TYR:CZ	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:ILE:HD12	1:F:174:ILE:CD1	2.15	0.77
1:F:77:ASN:H	1:F:77:ASN:HD22	1.31	0.77
1:C:407:TYR:HB3	5:C:1004:HOH:O	1.84	0.77
1:A:338:ILE:HG22	1:A:447:VAL:CG1	2.15	0.77
1:C:116:VAL:HG22	1:C:127:ILE:HG21	1.65	0.76
1:D:127:ILE:CG2	5:D:1080:HOH:O	2.33	0.76
1:F:66:ALA:C	1:F:68:GLN:H	1.93	0.76
1:F:55:ASN:H	1:F:77:ASN:ND2	1.82	0.76
1:F:126:PRO:HG3	1:F:145:LYS:HE3	1.65	0.76
1:C:453:GLN:HE21	1:C:457:GLU:CG	1.98	0.76
1:F:196:ILE:HG12	1:F:329:ILE:HD11	1.68	0.76
1:A:397:TRP:CE3	1:A:409:MSE:HE1	2.20	0.76
1:E:213:THR:HG21	1:E:215:TYR:CZ	2.20	0.75
1:F:131:THR:HG22	1:F:170:THR:OG1	1.85	0.75
1:F:311:ALA:HB2	1:F:342:PRO:HG3	1.67	0.75
1:F:39:LEU:HB3	1:F:74:VAL:HG21	1.68	0.75
1:F:53:LEU:CD2	1:F:222:ILE:CD1	2.60	0.75
1:E:60:ILE:HB	1:E:208:PRO:HD3	1.68	0.75
1:D:59:THR:HG23	5:D:1038:HOH:O	1.87	0.74
1:F:207:ASP:OD2	1:F:211:ASN:HB2	1.87	0.74
1:E:221:LYS:HE2	5:E:1045:HOH:O	1.86	0.74
1:F:117:LEU:CD2	1:F:148:ILE:HD13	2.14	0.74
1:F:127:ILE:CD1	1:F:174:ILE:HD13	2.18	0.74
1:A:224:LYS:HD2	5:A:1026:HOH:O	1.88	0.74
1:C:390:LYS:HE2	1:C:437:GLU:OE2	1.88	0.74
1:D:280:LYS:HG3	5:D:1089:HOH:O	1.88	0.74
1:F:58:ILE:HG12	1:F:74:VAL:HG22	1.70	0.74
1:B:381:TYR:HB2	1:B:428:GLU:HG3	1.69	0.73
1:A:338:ILE:HG22	1:A:447:VAL:HG13	1.70	0.73
1:F:422:TYR:CG	1:F:427:LYS:HB3	2.22	0.73
1:D:127:ILE:HG23	5:D:1080:HOH:O	1.87	0.73
1:F:289:THR:HG22	1:F:292:GLU:CD	2.13	0.73
1:C:127:ILE:CG1	1:C:144:LEU:HD12	2.19	0.73
1:F:117:LEU:CD2	1:F:148:ILE:CD1	2.66	0.73
1:F:207:ASP:HB2	1:F:208:PRO:HD2	1.70	0.73
1:A:120:GLN:HE22	1:A:146:ILE:N	1.86	0.73
1:D:338:ILE:HG12	1:D:447:VAL:HG13	1.70	0.73
1:E:38:GLU:OE2	5:E:976:HOH:O	2.06	0.73
1:C:127:ILE:CG1	1:C:144:LEU:CD1	2.66	0.73
1:F:422:TYR:CD1	1:F:427:LYS:HB3	2.23	0.73
1:F:24:GLY:C	1:F:26:PRO:HD3	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:THR:HG23	1:F:256:GLU:CB	2.19	0.72
1:C:120:GLN:NE2	1:C:146:ILE:H	1.85	0.72
1:B:390:LYS:HE3	1:B:394:GLU:OE2	1.89	0.72
1:C:332:PRO:HA	1:C:359:GLY:O	1.89	0.72
1:F:425:ALA:C	1:F:427:LYS:H	1.97	0.72
5:C:950:HOH:O	1:D:6:LYS:HD3	1.89	0.72
1:E:37:ARG:HH11	1:E:37:ARG:HG2	1.54	0.72
1:F:245:ILE:HG22	1:F:246:ASN:H	1.54	0.72
1:F:358:PHE:CG	1:F:358:PHE:O	2.41	0.72
1:B:226:PRO:HG3	1:B:315:SER:HB2	1.72	0.72
1:F:37:ARG:HG3	1:F:190:TYR:CE1	2.23	0.72
1:C:441:LYS:HE2	1:C:445:MSE:CE	2.20	0.72
1:E:192:LYS:CE	5:E:1044:HOH:O	2.38	0.72
1:C:207:ASP:HB2	1:C:208:PRO:CD	2.19	0.72
1:F:192:LYS:HG3	5:F:985:HOH:O	1.89	0.72
1:C:123:GLN:HE22	1:C:125:LYS:HB2	1.55	0.71
1:F:253:THR:CG2	1:F:256:GLU:CG	2.67	0.71
1:A:192:LYS:HE2	5:A:1033:HOH:O	1.90	0.71
1:B:453:GLN:HE21	1:B:457:GLU:HG3	1.56	0.71
1:C:107:MSE:HE1	1:C:420:ILE:H	1.56	0.71
1:D:368:PRO:HG3	1:D:409:MSE:HE3	1.70	0.71
1:F:54:PRO:HB2	1:F:201:ALA:HB1	1.73	0.71
1:C:229:VAL:HG11	1:C:313:SER:HB3	1.72	0.71
1:F:36:VAL:O	1:F:40:ILE:HD13	1.91	0.71
1:F:264:SER:HA	1:F:307:ARG:HH11	1.55	0.71
1:A:137:LYS:HD2	1:A:137:LYS:N	2.02	0.71
1:C:368:PRO:HG3	1:C:409:MSE:HE3	1.71	0.70
1:F:130:GLU:HB2	1:F:171:SER:HB3	1.71	0.70
1:D:21:GLU:H	1:D:21:GLU:CD	1.99	0.70
1:E:37:ARG:HG3	1:E:37:ARG:NH1	2.06	0.70
1:D:116:VAL:HG22	1:D:127:ILE:HG21	1.74	0.70
1:F:245:ILE:O	1:F:247:ASN:N	2.24	0.70
1:F:398:LYS:O	1:F:400:TYR:N	2.25	0.70
1:C:17:LYS:HZ2	1:C:121:MSE:HE3	1.56	0.70
1:E:167:PHE:HA	5:E:1062:HOH:O	1.90	0.70
1:F:195:TYR:HA	1:F:198:THR:HG22	1.74	0.70
1:F:340:ARG:HD3	1:F:439:GLU:OE2	1.90	0.70
1:B:240:GLU:HA	5:B:1054:HOH:O	1.91	0.70
1:E:163:ASN:ND2	1:E:167:PHE:HB3	2.06	0.69
1:C:127:ILE:HD11	1:C:144:LEU:HD11	0.75	0.69
1:F:86:VAL:N	1:F:87:PRO:CD	2.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASN:ND2	1:A:30:ARG:H	1.89	0.69
1:B:77:ASN:O	1:B:168:HIS:CE1	2.46	0.69
1:C:223:PRO:O	1:C:224:LYS:C	2.35	0.69
1:F:42:ASN:ND2	5:F:982:HOH:O	2.16	0.69
1:F:194:THR:CG2	5:F:975:HOH:O	2.41	0.69
1:F:296:LEU:HD21	1:F:300:PHE:CZ	2.28	0.69
1:C:407:TYR:CD2	1:C:409:MSE:HE2	2.28	0.69
1:F:110:LEU:HD13	1:F:110:LEU:N	2.08	0.69
1:F:207:ASP:O	1:F:209:GLU:N	2.26	0.69
1:F:245:ILE:O	1:F:246:ASN:C	2.35	0.69
1:C:330:PHE:HA	5:C:945:HOH:O	1.92	0.68
1:F:141:THR:OG1	1:F:159:GLY:CA	2.41	0.68
1:F:83:PRO:CG	1:F:140:TYR:CE2	2.75	0.68
1:F:408:GLN:HB3	5:F:1015:HOH:O	1.92	0.68
1:A:4:LYS:CG	5:B:962:HOH:O	2.23	0.68
1:A:252:TYR:O	1:A:285:VAL:HG23	1.93	0.68
1:D:252:TYR:O	1:D:285:VAL:HG23	1.94	0.68
1:F:110:LEU:N	1:F:110:LEU:CD1	2.56	0.68
1:B:387:VAL:HG11	1:B:432:GLU:HA	1.74	0.68
1:E:192:LYS:HE3	5:E:1044:HOH:O	1.93	0.68
1:E:279:LEU:HD21	1:E:292:GLU:HB3	1.76	0.68
1:D:30:ARG:HD2	5:D:1022:HOH:O	1.93	0.68
1:F:127:ILE:CD1	1:F:174:ILE:CD1	2.72	0.67
1:F:4:LYS:HG3	5:F:1016:HOH:O	1.94	0.67
1:F:54:PRO:HB2	1:F:201:ALA:CB	2.25	0.67
1:D:340:ARG:HD3	1:D:439:GLU:OE2	1.95	0.67
1:D:364:VAL:HG12	1:D:406:GLN:HG2	1.76	0.67
1:B:322:ILE:HG23	1:B:412:MSE:CE	2.25	0.67
1:E:405:ASP:OD1	1:E:406:GLN:N	2.27	0.67
1:F:226:PRO:HG3	1:F:315:SER:HB3	1.74	0.67
1:C:251:ASP:OD1	1:C:284:LYS:HD2	1.95	0.67
1:F:207:ASP:CG	1:F:211:ASN:HB2	2.20	0.67
1:B:107:MSE:HE2	1:B:108:TYR:CE1	2.30	0.66
1:F:203:PHE:HB2	1:F:215:TYR:CB	2.20	0.66
1:F:253:THR:CG2	1:F:256:GLU:HB2	2.25	0.66
1:F:289:THR:HG23	1:F:292:GLU:H	1.59	0.66
1:C:249:LYS:HA	1:C:249:LYS:CE	2.25	0.66
1:F:83:PRO:HG3	1:F:140:TYR:CD2	2.30	0.66
1:F:54:PRO:O	1:F:202:GLU:N	2.26	0.66
1:B:150:LYS:HE3	5:B:996:HOH:O	1.95	0.66
1:C:229:VAL:HG11	1:C:313:SER:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:ILE:C	1:F:199:PRO:HD3	2.20	0.66
1:F:358:PHE:O	1:F:358:PHE:CD2	2.49	0.66
1:F:53:LEU:HD21	1:F:222:ILE:HG13	1.78	0.65
1:B:259:VAL:HG23	1:B:260:ASN:OD1	1.96	0.65
1:D:348:HIS:HB3	1:D:418:THR:HG22	1.77	0.65
1:A:125:LYS:HD3	5:A:1023:HOH:O	1.95	0.65
1:F:243:ILE:O	1:F:247:ASN:HB2	1.97	0.65
1:A:92:ARG:O	1:A:113:LYS:HE3	1.97	0.65
1:E:277:ALA:HB2	1:E:299:THR:HG21	1.78	0.65
1:C:121:MSE:CE	1:D:237:ASP:OD2	2.45	0.65
1:C:407:TYR:CE2	1:C:409:MSE:CE	2.80	0.65
1:E:453:GLN:HE21	1:E:457:GLU:HG3	1.60	0.65
1:F:219:THR:CG2	1:F:221:LYS:HB3	2.26	0.65
1:F:408:GLN:C	5:F:1015:HOH:O	2.40	0.65
1:A:123:GLN:HE22	1:A:125:LYS:HB2	1.60	0.65
1:F:86:VAL:H	1:F:87:PRO:CD	2.10	0.65
1:E:391:VAL:HG13	1:E:441:LYS:HG2	1.79	0.65
1:F:39:LEU:CB	1:F:74:VAL:HG21	2.27	0.64
1:F:391:VAL:HG11	1:F:440:ILE:HG22	1.79	0.64
1:B:134:VAL:HG12	1:B:134:VAL:O	1.96	0.64
1:C:453:GLN:NE2	1:C:457:GLU:CG	2.60	0.64
1:F:255:LYS:HE2	5:F:970:HOH:O	1.98	0.64
1:A:330:PHE:O	1:A:361:SER:HB2	1.96	0.64
1:F:330:PHE:C	1:F:332:PRO:CD	2.71	0.64
1:F:387:VAL:HG12	1:F:430:ILE:HB	1.79	0.64
1:D:280:LYS:CG	5:D:1089:HOH:O	2.44	0.64
1:A:345:TYR:CG	1:A:436:ILE:HD11	2.33	0.64
1:D:89:ALA:O	1:D:113:LYS:HE3	1.98	0.64
1:D:100:VAL:HG13	1:D:228:GLU:CD	2.23	0.64
1:D:364:VAL:CG1	1:D:406:GLN:HG2	2.28	0.64
1:F:118:TYR:HA	1:F:121:MSE:HE2	1.81	0.64
1:D:250:ARG:HG2	1:D:250:ARG:NH1	2.07	0.63
1:E:192:LYS:HD2	5:E:1050:HOH:O	1.97	0.63
1:D:257:PHE:HB2	1:D:285:VAL:HG21	1.81	0.63
1:D:179:ASP:OD2	1:D:182:LYS:CD	2.45	0.63
1:F:180:TRP:HB3	1:F:181:PRO:HD3	1.79	0.63
1:A:123:GLN:NE2	1:A:125:LYS:HB2	2.14	0.63
1:C:441:LYS:HE2	1:C:445:MSE:HE1	1.81	0.63
1:C:121:MSE:HE3	1:D:237:ASP:OD2	1.98	0.63
3:F:950:ANP:C2'	5:F:951:HOH:O	2.43	0.63
1:E:53:LEU:HD23	1:E:222:ILE:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:LEU:HD21	1:E:328:LYS:HE3	1.80	0.63
1:F:58:ILE:HA	1:F:73:ASN:O	1.97	0.63
1:A:206:LYS:HE2	5:A:981:HOH:O	1.98	0.63
1:C:17:LYS:HZ3	1:C:121:MSE:HE3	1.64	0.63
1:A:460:LYS:HD2	5:A:998:HOH:O	1.99	0.63
1:B:248:LEU:HD22	1:B:252:TYR:CE2	2.34	0.63
1:D:207:ASP:HB2	1:D:208:PRO:CD	2.28	0.63
1:E:120:GLN:HE22	1:E:146:ILE:H	0.77	0.62
1:F:34:GLN:O	1:F:38:GLU:HG2	1.99	0.62
1:F:35:THR:O	1:F:39:LEU:HG	1.98	0.62
1:A:120:GLN:NE2	1:A:146:ILE:H	1.92	0.62
1:D:4:LYS:N	5:D:997:HOH:O	2.31	0.62
1:F:368:PRO:HG3	1:F:409:MSE:HE3	1.81	0.62
1:D:255:LYS:NZ	1:D:267:ASP:OD1	2.32	0.62
1:F:18:ARG:C	1:F:20:PRO:HD3	2.24	0.62
1:F:57:LYS:HB3	1:F:204:ILE:HB	1.82	0.62
1:A:167:PHE:N	5:A:1054:HOH:O	2.32	0.62
1:C:240:GLU:HG3	1:D:17:LYS:HE3	1.82	0.62
1:A:222:ILE:HG13	1:A:223:PRO:HD2	1.82	0.62
1:B:387:VAL:CG1	1:B:432:GLU:HA	2.29	0.62
1:C:221:LYS:HD2	1:C:222:ILE:N	2.14	0.62
1:F:408:GLN:CA	5:F:1015:HOH:O	2.47	0.62
1:A:292:GLU:HG2	1:A:295:ARG:HH21	1.64	0.62
1:F:149:ASN:N	5:F:969:HOH:O	2.31	0.62
1:F:426:GLY:C	1:F:427:LYS:HG3	2.24	0.62
1:F:139:ILE:HG22	1:F:139:ILE:O	2.00	0.62
1:F:53:LEU:CG	1:F:222:ILE:HD11	2.30	0.61
1:F:289:THR:OG1	1:F:291:GLU:HG2	2.00	0.61
1:B:139:ILE:CG1	1:B:163:ASN:HB3	2.26	0.61
1:B:240:GLU:CA	5:B:1054:HOH:O	2.48	0.61
1:D:17:LYS:HD3	1:D:17:LYS:C	2.25	0.61
1:D:92:ARG:O	1:D:113:LYS:HE2	2.00	0.61
1:C:127:ILE:HG12	1:C:144:LEU:HD12	1.81	0.61
1:C:340:ARG:HD3	1:C:439:GLU:OE2	2.00	0.61
1:E:318:GLY:O	1:E:322:ILE:HG13	1.98	0.61
1:C:423:LYS:HZ1	1:D:382:ASP:CG	2.08	0.61
1:D:292:GLU:HG2	1:D:295:ARG:NH2	2.16	0.61
1:B:150:LYS:NZ	5:B:996:HOH:O	2.34	0.61
1:B:232:HIS:O	1:B:347:GLY:HA2	1.99	0.61
1:E:398:LYS:HD2	5:E:1005:HOH:O	1.99	0.61
1:F:33:TYR:CD2	1:F:33:TYR:O	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:LEU:HD23	1:F:222:ILE:CG1	2.30	0.61
1:C:123:GLN:NE2	1:C:125:LYS:HB2	2.16	0.61
1:E:14:GLU:CG	1:E:148:ILE:HG22	2.31	0.61
1:A:26:PRO:HD2	1:A:30:ARG:HG2	1.83	0.61
1:A:403:GLU:CG	1:A:404:SER:H	2.07	0.61
1:F:4:LYS:HE3	5:F:991:HOH:O	2.01	0.60
1:F:53:LEU:CD2	1:F:222:ILE:CG1	2.79	0.60
1:F:206:LYS:CG	1:F:211:ASN:O	2.48	0.60
1:F:227:GLN:HB2	5:F:976:HOH:O	2.01	0.60
1:F:253:THR:HG23	1:F:256:GLU:H	1.65	0.60
1:C:390:LYS:O	1:C:394:GLU:HG3	2.01	0.60
1:E:419:LYS:NZ	1:F:18:ARG:O	2.31	0.60
1:A:343:LYS:HE2	5:A:950:HOH:O	2.00	0.60
1:B:269:THR:O	1:B:273:ILE:HG12	2.01	0.60
1:C:50:HIS:CD2	1:C:79:ILE:HD13	2.36	0.60
1:C:238:ARG:HH22	1:C:290:GLU:CG	1.97	0.60
1:A:6:LYS:O	1:B:97:SER:HA	2.01	0.60
1:F:86:VAL:N	1:F:87:PRO:HD2	2.16	0.60
1:F:253:THR:OG1	1:F:282:ASN:HA	2.01	0.60
1:A:400:TYR:OH	1:A:445:MSE:HG2	2.01	0.60
1:A:445:MSE:O	1:A:449:ARG:HD3	2.01	0.60
1:E:24:GLY:C	1:E:26:PRO:HD3	2.27	0.60
1:F:245:ILE:O	1:F:248:LEU:N	2.31	0.60
1:E:48:ASP:OD1	1:E:105:ARG:NH2	2.30	0.60
1:F:86:VAL:H	1:F:87:PRO:HD2	1.66	0.60
1:F:196:ILE:CG1	1:F:329:ILE:HD11	2.32	0.60
1:A:316:VAL:CG1	1:A:353:GLU:OE2	2.50	0.60
1:F:339:THR:O	1:F:339:THR:HG22	2.01	0.60
1:F:253:THR:HG23	1:F:256:GLU:HG3	1.84	0.59
1:B:43:SER:HB3	1:B:76:ASP:HB3	1.84	0.59
1:E:8:THR:HG23	1:F:99:TYR:HD2	1.67	0.59
1:E:295:ARG:NH1	5:E:1054:HOH:O	2.33	0.59
1:A:123:GLN:NE2	1:A:125:LYS:N	2.49	0.59
1:F:37:ARG:HG3	1:F:190:TYR:CZ	2.37	0.59
1:F:433:VAL:HB	1:F:436:ILE:HD12	1.85	0.59
1:B:453:GLN:HE21	1:B:457:GLU:CG	2.16	0.59
1:F:289:THR:HG23	1:F:292:GLU:N	2.18	0.59
1:B:240:GLU:HB3	5:B:1054:HOH:O	2.03	0.59
1:F:400:TYR:OH	1:F:445:MSE:HG2	2.03	0.59
1:C:221:LYS:HD2	1:C:221:LYS:C	2.27	0.59
1:A:322:ILE:HG12	1:A:412:MSE:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLU:HG2	1:A:404:SER:N	2.07	0.59
1:D:366:GLU:HG2	5:D:1058:HOH:O	2.02	0.59
1:C:407:TYR:HE2	1:C:409:MSE:HE1	1.68	0.58
1:D:404:SER:C	1:D:406:GLN:H	2.11	0.58
1:F:228:GLU:HB2	5:F:999:HOH:O	2.02	0.58
1:F:66:ALA:C	1:F:68:GLN:N	2.58	0.58
1:E:397:TRP:C	1:E:399:ARG:H	2.11	0.58
1:C:207:ASP:HB2	1:C:208:PRO:HD3	1.86	0.57
1:E:5:GLU:N	5:E:1037:HOH:O	2.36	0.57
1:F:30:ARG:HD2	1:F:381:TYR:CE1	2.39	0.57
1:F:311:ALA:HB2	1:F:342:PRO:HG2	1.86	0.57
1:A:135:ASN:CG	5:A:978:HOH:O	2.47	0.57
1:A:207:ASP:HB2	1:A:208:PRO:CD	2.34	0.57
1:C:21:GLU:CD	1:C:21:GLU:H	2.12	0.57
1:C:123:GLN:NE2	1:C:125:LYS:H	2.02	0.57
1:D:399:ARG:CD	5:D:1018:HOH:O	2.53	0.57
1:F:77:ASN:HD22	1:F:77:ASN:N	1.96	0.57
1:D:250:ARG:HG3	1:D:250:ARG:NH1	2.11	0.57
1:D:301:LYS:HG3	5:D:1064:HOH:O	2.03	0.57
1:F:212:VAL:HG11	1:F:214:TYR:HE1	1.68	0.57
1:C:226:PRO:HA	5:C:1058:HOH:O	2.03	0.57
1:F:214:TYR:HB3	1:F:216:PRO:HD3	1.87	0.57
1:F:401:GLY:O	1:F:402:ILE:C	2.47	0.57
1:F:238:ARG:HG2	1:F:293:ILE:HG22	1.87	0.57
1:B:375:ASN:O	1:B:376:LYS:HB2	2.04	0.57
1:A:320:ASP:O	1:A:324:LEU:HB2	2.03	0.57
1:F:217:ARG:NH2	1:F:220:ASN:HD21	2.02	0.57
1:A:4:LYS:CD	1:A:4:LYS:C	2.67	0.56
1:B:134:VAL:O	1:B:134:VAL:CG1	2.53	0.56
1:F:133:PRO:O	1:F:134:VAL:HG13	2.05	0.56
1:F:158:ARG:HG3	5:F:1013:HOH:O	2.05	0.56
1:A:250:ARG:HB2	1:A:252:TYR:CE1	2.40	0.56
1:D:192:LYS:HD2	5:D:1056:HOH:O	2.04	0.56
1:C:322:ILE:CG2	1:C:412:MSE:CE	2.76	0.56
1:A:24:GLY:C	1:A:26:PRO:HD3	2.30	0.56
1:C:365:GLY:O	1:C:407:TYR:HB2	2.05	0.56
1:D:383:GLU:HB2	5:D:983:HOH:O	2.05	0.56
1:E:86:VAL:HB	1:E:87:PRO:HD3	1.88	0.56
1:D:276:LEU:HD22	5:D:991:HOH:O	2.05	0.56
1:F:89:ALA:O	1:F:113:LYS:HE3	2.06	0.56
1:F:198:THR:N	1:F:199:PRO:HD3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:ASP:OD1	1:F:388:ILE:N	2.31	0.56
1:B:126:PRO:HD2	5:B:1047:HOH:O	2.05	0.56
1:B:427:LYS:NZ	3:B:910:ANP:O3G	2.26	0.56
1:F:126:PRO:HB3	1:F:144:LEU:O	2.05	0.56
1:F:404:SER:C	1:F:406:GLN:H	2.14	0.56
1:B:120:GLN:HE22	1:B:146:ILE:H	0.81	0.56
1:A:337:SER:HA	1:A:355:GLY:HA2	1.88	0.56
1:F:33:TYR:OH	1:F:380:ILE:HG12	2.05	0.56
1:F:194:THR:O	1:F:198:THR:HB	2.06	0.56
1:F:242:LYS:NZ	1:F:290:GLU:OE2	2.33	0.56
1:F:49:VAL:HG12	1:F:49:VAL:O	2.07	0.55
1:F:236:VAL:CG1	1:F:300:PHE:HD2	2.19	0.55
1:F:375:ASN:OD1	1:F:416:CYS:HA	2.05	0.55
1:B:242:LYS:NZ	1:B:290:GLU:OE2	2.38	0.55
1:F:327:LYS:HA	1:F:332:PRO:CD	2.32	0.55
1:B:250:ARG:NH1	1:B:252:TYR:CE1	2.73	0.55
1:C:249:LYS:HE2	1:C:249:LYS:CA	2.18	0.55
1:E:30:ARG:NH1	5:E:1016:HOH:O	2.34	0.55
1:F:81:ILE:HD13	1:F:90:PHE:HE2	1.72	0.55
1:C:385:SER:HB3	1:D:385:SER:OG	2.06	0.55
1:F:77:ASN:H	1:F:77:ASN:ND2	2.03	0.55
1:F:148:ILE:C	5:F:969:HOH:O	2.49	0.55
1:F:215:TYR:N	1:F:216:PRO:HD3	2.22	0.55
1:A:143:LYS:HB2	1:A:157:GLU:HB2	1.88	0.55
1:F:330:PHE:O	1:F:332:PRO:CD	2.54	0.55
1:A:312:ASP:OD1	1:A:312:ASP:C	2.50	0.55
1:B:102:ARG:HA	5:B:1034:HOH:O	2.06	0.55
1:C:407:TYR:HD2	1:C:409:MSE:HE2	1.71	0.55
1:D:193:ARG:HD2	5:D:1081:HOH:O	2.06	0.55
1:F:21:GLU:H	1:F:21:GLU:CD	2.15	0.55
1:F:264:SER:HA	1:F:307:ARG:NH1	2.20	0.55
1:B:202:GLU:OE2	1:B:214:TYR:OH	2.24	0.55
1:C:127:ILE:HD12	1:C:129:ILE:HD11	1.89	0.55
1:C:441:LYS:HE2	1:C:445:MSE:HE3	1.88	0.55
1:D:19:ASN:HB3	1:D:22:LEU:HD22	1.87	0.55
1:F:19:ASN:HB2	1:F:22:LEU:HD22	1.88	0.55
1:F:215:TYR:N	1:F:216:PRO:CD	2.70	0.55
1:A:117:LEU:O	1:A:121:MSE:HG3	2.06	0.55
1:B:180:TRP:HB3	1:B:181:PRO:HD3	1.88	0.55
1:C:93:VAL:HG12	1:C:94:LEU:HG	1.89	0.55
1:E:295:ARG:HG3	1:F:67:ARG:HH22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:THR:CG2	1:F:256:GLU:CB	2.84	0.55
1:F:330:PHE:N	1:F:330:PHE:CD2	2.74	0.55
1:A:332:PRO:HG2	1:A:357:ALA:HB1	1.88	0.54
1:E:121:MSE:O	1:F:237:ASP:HB2	2.07	0.54
1:A:328:LYS:HG3	5:A:1059:HOH:O	2.07	0.54
1:B:25:PHE:N	1:B:26:PRO:HD3	2.22	0.54
1:B:83:PRO:HG3	1:B:140:TYR:CE2	2.42	0.54
1:C:99:TYR:CE2	1:D:10:LEU:HG	2.42	0.54
1:E:402:ILE:HG22	1:E:403:GLU:C	2.24	0.54
1:A:395:LEU:HD11	1:A:445:MSE:HE3	1.90	0.54
1:F:130:GLU:O	1:F:170:THR:HA	2.07	0.54
1:D:158:ARG:HG2	1:D:159:GLY:N	2.21	0.54
1:A:99:TYR:HD2	1:B:8:THR:HG23	1.72	0.54
1:C:407:TYR:HE2	1:C:409:MSE:CE	2.18	0.54
1:E:14:GLU:HG2	1:E:148:ILE:HG22	1.89	0.54
1:F:110:LEU:HD13	1:F:110:LEU:H	1.72	0.54
1:B:250:ARG:NH1	1:B:252:TYR:OH	2.41	0.54
1:C:143:LYS:HB2	1:C:157:GLU:HB2	1.90	0.54
1:A:167:PHE:HB3	5:A:1036:HOH:O	2.06	0.54
1:A:284:LYS:HD3	1:A:286:LYS:HE2	1.89	0.54
1:E:30:ARG:HG3	5:E:1016:HOH:O	2.08	0.54
1:E:402:ILE:CG2	1:E:403:GLU:O	2.27	0.54
1:F:214:TYR:C	1:F:216:PRO:HD3	2.33	0.54
1:F:54:PRO:HD2	1:F:200:TYR:O	2.08	0.53
1:D:334:PHE:HA	5:D:1057:HOH:O	2.08	0.53
1:E:250:ARG:HD3	1:E:252:TYR:HE1	1.72	0.53
1:B:150:LYS:CE	5:B:996:HOH:O	2.53	0.53
1:B:358:PHE:O	1:B:358:PHE:CG	2.61	0.53
1:E:207:ASP:OD1	1:E:207:ASP:C	2.51	0.53
1:F:362:ILE:CB	5:F:1015:HOH:O	2.56	0.53
1:E:14:GLU:HG3	1:E:148:ILE:HG22	1.91	0.53
1:A:190:TYR:O	1:A:194:THR:HG22	2.08	0.53
1:F:255:LYS:O	1:F:259:VAL:HG13	2.08	0.53
1:F:318:GLY:O	1:F:322:ILE:HG13	2.09	0.53
1:F:425:ALA:C	1:F:427:LYS:N	2.64	0.53
1:A:161:VAL:CG1	1:A:162:GLU:N	2.71	0.53
1:C:65:ASP:C	1:C:65:ASP:OD1	2.52	0.53
1:D:255:LYS:CE	1:D:267:ASP:OD1	2.56	0.53
1:A:340:ARG:HD3	1:A:439:GLU:OE2	2.09	0.53
1:B:441:LYS:CE	1:B:445:MSE:CE	2.73	0.53
1:F:127:ILE:HD11	1:F:172:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASN:H	1:A:332:PRO:HD3	1.73	0.53
1:C:331:ASN:CG	1:C:331:ASN:O	2.52	0.53
1:E:93:VAL:HG12	1:E:94:LEU:HG	1.91	0.53
1:B:331:ASN:N	1:B:332:PRO:HD3	2.24	0.53
1:F:42:ASN:HB3	3:F:950:ANP:N7	2.24	0.53
1:B:397:TRP:C	1:B:399:ARG:H	2.17	0.52
1:A:257:PHE:HB2	1:A:285:VAL:HG21	1.91	0.52
1:D:326:LEU:HD21	1:D:412:MSE:HG2	1.90	0.52
1:E:21:GLU:CD	1:E:21:GLU:H	2.17	0.52
1:E:89:ALA:O	1:E:113:LYS:HE2	2.09	0.52
1:F:42:ASN:O	5:F:1029:HOH:O	2.19	0.52
1:F:245:ILE:CG2	1:F:246:ASN:N	2.68	0.52
1:A:331:ASN:N	1:A:332:PRO:CD	2.71	0.52
1:C:161:VAL:HG12	1:C:162:GLU:N	2.24	0.52
1:F:253:THR:HG23	1:F:256:GLU:CG	2.37	0.52
1:F:301:LYS:HD3	5:F:1001:HOH:O	2.08	0.52
1:B:207:ASP:HB2	1:B:208:PRO:CD	2.39	0.52
1:C:322:ILE:HG23	1:C:412:MSE:HE1	1.85	0.52
1:C:71:LYS:NZ	5:C:979:HOH:O	2.40	0.52
1:C:453:GLN:HE21	1:C:457:GLU:CD	2.17	0.52
1:E:180:TRP:HB3	1:E:181:PRO:HD3	1.92	0.52
1:D:112:VAL:HG12	3:D:930:ANP:O2A	2.10	0.52
1:E:311:ALA:CB	1:E:342:PRO:CG	2.82	0.52
1:A:10:LEU:HG	1:B:99:TYR:CE2	2.45	0.52
1:C:45:ASP:O	1:C:49:VAL:HB	2.10	0.52
1:E:10:LEU:HG	1:F:99:TYR:CE2	2.44	0.52
1:F:194:THR:HG21	5:F:975:HOH:O	2.09	0.52
1:D:34:GLN:O	1:D:38:GLU:HG2	2.10	0.52
1:F:141:THR:HG1	1:F:159:GLY:HA3	1.71	0.52
1:A:47:THR:HG22	1:A:78:GLY:HA2	1.92	0.52
1:A:273:ILE:HD11	1:A:306:PHE:CE1	2.44	0.52
1:F:192:LYS:HE2	5:F:1011:HOH:O	2.10	0.52
1:F:229:VAL:HG11	1:F:313:SER:CB	2.37	0.52
1:F:253:THR:OG1	1:F:281:PRO:O	2.27	0.52
1:A:436:ILE:N	1:A:436:ILE:HD12	2.24	0.52
1:B:64:ASP:OD2	1:B:67:ARG:HD2	2.10	0.52
1:C:92:ARG:O	1:C:113:LYS:HD2	2.10	0.52
1:C:453:GLN:NE2	1:C:457:GLU:OE2	2.43	0.51
1:F:330:PHE:O	1:F:332:PRO:HD3	2.10	0.51
1:B:34:GLN:O	1:B:38:GLU:HG2	2.10	0.51
1:E:77:ASN:O	1:E:168:HIS:CE1	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:ALA:CB	1:E:342:PRO:HG3	2.40	0.51
1:F:327:LYS:HA	1:F:332:PRO:HG2	1.92	0.51
1:E:324:LEU:CD2	1:E:328:LYS:HE3	2.41	0.51
1:B:248:LEU:HD22	1:B:252:TYR:CD2	2.46	0.51
1:A:232:HIS:CG	1:A:233:PRO:HD2	2.46	0.51
1:B:358:PHE:O	1:B:358:PHE:CD2	2.64	0.51
1:C:407:TYR:CE2	1:C:409:MSE:HE2	2.43	0.51
1:D:400:TYR:O	1:D:452:LYS:HG3	2.10	0.51
1:C:132:SER:O	1:C:168:HIS:HA	2.10	0.51
1:F:194:THR:HG23	5:F:975:HOH:O	2.06	0.51
1:F:395:LEU:HD22	1:F:444:LEU:HD13	1.92	0.51
1:C:144:LEU:HD12	1:C:144:LEU:C	2.36	0.51
1:F:219:THR:HG23	1:F:221:LYS:H	1.76	0.51
1:B:427:LYS:NZ	5:B:998:HOH:O	2.44	0.51
1:E:258:LEU:HD11	1:E:274:LEU:HD21	1.92	0.51
1:E:303:TYR:CE2	1:E:305:ASP:HB2	2.46	0.51
1:D:127:ILE:HG22	5:D:1080:HOH:O	2.06	0.50
1:E:192:LYS:HE2	5:E:996:HOH:O	2.09	0.50
1:A:5:GLU:OE2	1:B:50:HIS:NE2	2.45	0.50
1:D:130:GLU:HG2	1:D:141:THR:HG22	1.92	0.50
1:A:422:TYR:CD2	1:A:427:LYS:HD2	2.47	0.50
1:C:232:HIS:O	1:C:347:GLY:HA2	2.11	0.50
1:D:263:GLN:O	1:D:264:SER:HB2	2.10	0.50
1:A:93:VAL:HG13	1:A:110:LEU:HD23	1.94	0.50
1:E:254:ILE:O	1:E:258:LEU:HG	2.12	0.50
1:A:375:ASN:OD1	1:A:416:CYS:HA	2.11	0.50
1:F:25:PHE:N	1:F:26:PRO:HD3	2.27	0.50
1:F:253:THR:HG22	1:F:256:GLU:OE1	2.11	0.50
1:A:391:VAL:HG13	1:A:441:LYS:HG2	1.93	0.50
1:A:407:TYR:N	1:A:407:TYR:CD2	2.80	0.50
1:C:331:ASN:N	1:C:332:PRO:HD3	2.27	0.50
1:E:250:ARG:HD3	1:E:252:TYR:CE1	2.47	0.50
1:F:233:PRO:HG3	1:F:265:ILE:HD11	1.94	0.50
1:F:253:THR:HG21	1:F:256:GLU:HG3	1.89	0.50
1:A:6:LYS:NZ	1:B:228:GLU:OE1	2.42	0.49
1:A:409:MSE:HB2	5:A:1021:HOH:O	2.10	0.49
1:D:96:SER:HB2	1:D:109:GLY:CA	2.42	0.49
1:E:398:LYS:HG2	1:E:402:ILE:O	2.12	0.49
1:A:123:GLN:HE22	1:A:125:LYS:CB	2.25	0.49
1:A:232:HIS:ND1	1:A:233:PRO:HD2	2.27	0.49
1:F:4:LYS:CG	5:F:1016:HOH:O	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:TRP:CD1	1:F:208:PRO:HG2	2.44	0.49
1:F:232:HIS:CD2	1:F:309:PRO:HG3	2.47	0.49
1:A:365:GLY:O	1:A:406:GLN:HA	2.12	0.49
1:A:402:ILE:HD12	1:A:455:LEU:HD11	1.94	0.49
1:A:127:ILE:HG13	1:A:174:ILE:HG12	1.93	0.49
1:D:193:ARG:CD	5:D:1081:HOH:O	2.59	0.49
1:B:207:ASP:HB2	1:B:208:PRO:HD2	1.95	0.49
1:E:398:LYS:HG3	1:E:404:SER:HB2	1.94	0.49
1:F:57:LYS:HA	1:F:204:ILE:O	2.13	0.49
1:B:92:ARG:O	1:B:113:LYS:HE3	2.13	0.49
1:E:193:ARG:O	1:E:196:ILE:HG13	2.13	0.49
1:F:53:LEU:CD2	1:F:222:ILE:HG13	2.42	0.49
1:B:196:ILE:HG23	1:B:197:ILE:HG23	1.94	0.49
1:C:427:LYS:NZ	5:C:955:HOH:O	2.24	0.49
1:F:188:TYR:HD1	5:F:985:HOH:O	1.95	0.49
1:D:255:LYS:HE2	1:D:267:ASP:OD1	2.13	0.49
1:B:453:GLN:NE2	1:B:457:GLU:HG3	2.25	0.49
1:D:100:VAL:CG1	1:D:228:GLU:CD	2.86	0.49
1:F:381:TYR:HB2	1:F:428:GLU:CG	2.37	0.49
1:A:459:ARG:O	1:A:462:GLN:N	2.46	0.49
1:B:167:PHE:HA	5:B:1050:HOH:O	2.12	0.49
1:B:284:LYS:HD3	1:B:286:LYS:HE2	1.94	0.49
1:C:207:ASP:HB2	1:C:208:PRO:HD2	1.95	0.49
1:F:423:LYS:NZ	1:F:432:GLU:OE2	2.37	0.49
1:D:370:VAL:O	1:D:371:LEU:HD12	2.13	0.48
1:E:92:ARG:O	1:E:113:LYS:HD3	2.13	0.48
1:F:52:ILE:O	1:F:54:PRO:HD3	2.13	0.48
1:A:461:GLU:HA	1:A:461:GLU:OE1	2.13	0.48
1:B:113:LYS:NZ	3:B:910:ANP:O2A	2.42	0.48
1:E:289:THR:HG23	1:E:292:GLU:HG3	1.94	0.48
1:E:402:ILE:HD12	1:E:402:ILE:N	2.28	0.48
1:F:128:GLU:HB2	1:F:173:ALA:HB3	1.94	0.48
1:C:205:PHE:O	1:C:212:VAL:HA	2.13	0.48
1:D:441:LYS:HZ1	1:D:445:MSE:HE1	1.79	0.48
1:D:383:GLU:HG3	5:D:1035:HOH:O	2.14	0.48
1:D:441:LYS:NZ	1:D:445:MSE:HE1	2.29	0.48
1:A:26:PRO:CD	1:A:30:ARG:HG2	2.42	0.48
1:C:254:ILE:HA	1:C:285:VAL:HG13	1.95	0.48
1:F:196:ILE:HG12	1:F:329:ILE:CD1	2.40	0.48
1:F:255:LYS:NZ	1:F:271:ASP:OD1	2.45	0.48
1:A:148:ILE:HD13	1:A:148:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PRO:HA	1:B:144:LEU:HD21	1.96	0.48
1:F:400:TYR:O	1:F:452:LYS:HG3	2.13	0.48
1:F:283:LYS:HG2	1:F:284:LYS:N	2.27	0.48
1:C:196:ILE:HG22	1:C:197:ILE:HG23	1.95	0.48
1:D:399:ARG:NE	5:D:1018:HOH:O	2.47	0.48
1:A:402:ILE:HG22	5:A:977:HOH:O	2.13	0.48
1:E:444:LEU:O	1:E:447:VAL:HG23	2.14	0.48
1:F:236:VAL:CG1	1:F:300:PHE:CD2	2.97	0.48
1:A:207:ASP:HB2	1:A:208:PRO:HD3	1.94	0.48
1:B:123:GLN:OE1	1:B:125:LYS:HB2	2.14	0.48
1:C:136:SER:HA	5:C:1044:HOH:O	2.13	0.48
1:E:21:GLU:OE2	1:F:419:LYS:NZ	2.44	0.48
1:F:33:TYR:O	1:F:33:TYR:CG	2.67	0.48
1:A:229:VAL:HG11	1:A:313:SER:CB	2.38	0.47
1:C:34:GLN:O	1:C:38:GLU:HG2	2.14	0.47
1:C:340:ARG:CD	1:C:439:GLU:OE2	2.61	0.47
1:A:96:SER:HB2	1:A:109:GLY:CA	2.44	0.47
1:A:338:ILE:CG2	1:A:447:VAL:HG13	2.40	0.47
1:B:193:ARG:O	1:B:196:ILE:HG22	2.13	0.47
1:C:124:ASP:HB2	5:C:983:HOH:O	2.14	0.47
1:E:49:VAL:HG12	1:E:49:VAL:O	2.13	0.47
1:F:317:ILE:O	1:F:321:LEU:HD12	2.14	0.47
1:A:255:LYS:NZ	1:A:271:ASP:OD1	2.32	0.47
1:A:316:VAL:HG12	1:A:318:GLY:N	2.29	0.47
1:C:44:LEU:HB3	1:C:105:ARG:CZ	2.43	0.47
1:E:30:ARG:HD3	1:E:381:TYR:CE1	2.48	0.47
1:F:33:TYR:CD2	1:F:381:TYR:HE2	2.31	0.47
1:F:219:THR:CG2	1:F:221:LYS:H	2.27	0.47
1:A:161:VAL:HG12	1:A:162:GLU:N	2.29	0.47
1:B:65:ASP:OD2	1:B:65:ASP:N	2.46	0.47
1:F:53:LEU:HD21	1:F:222:ILE:CG1	2.43	0.47
1:F:214:TYR:C	1:F:216:PRO:CD	2.87	0.47
1:F:373:TYR:HA	1:F:377:ILE:O	2.14	0.47
1:A:190:TYR:O	1:A:194:THR:CG2	2.63	0.47
1:E:37:ARG:NH1	1:E:41:GLU:OE1	2.47	0.47
1:A:99:TYR:CE2	1:B:10:LEU:HG	2.49	0.47
1:B:17:LYS:HG2	1:B:148:ILE:HD13	1.97	0.47
1:B:390:LYS:HG3	1:B:394:GLU:OE2	2.15	0.47
1:B:400:TYR:O	1:B:452:LYS:HA	2.15	0.47
1:F:4:LYS:HE2	5:F:1016:HOH:O	2.14	0.47
1:F:117:LEU:HD23	1:F:148:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:ALA:CB	1:F:342:PRO:HG3	2.43	0.47
1:F:398:LYS:O	1:F:399:ARG:C	2.56	0.47
1:A:26:PRO:HD2	1:A:30:ARG:CG	2.43	0.47
1:A:102:ARG:HD3	1:A:104:THR:CG2	2.44	0.47
1:A:123:GLN:NE2	1:A:125:LYS:CB	2.78	0.47
1:B:333:ASP:H	1:B:359:GLY:HA3	1.79	0.47
1:C:254:ILE:HG22	1:C:274:LEU:HD21	1.97	0.47
1:E:117:LEU:C	1:E:121:MSE:HE3	2.40	0.47
1:F:149:ASN:CA	5:F:969:HOH:O	2.62	0.47
1:F:232:HIS:CG	1:F:233:PRO:HD2	2.49	0.47
1:F:253:THR:HG22	1:F:256:GLU:CG	2.43	0.47
1:F:444:LEU:HD23	1:F:444:LEU:HA	1.64	0.47
1:A:423:LYS:HG2	1:A:431:ALA:HB2	1.95	0.47
1:B:47:THR:HG22	1:B:78:GLY:HA2	1.97	0.47
1:E:221:LYS:CE	5:E:1045:HOH:O	2.55	0.47
1:E:358:PHE:CD2	1:E:359:GLY:N	2.83	0.47
1:F:43:SER:O	1:F:46:ALA:N	2.48	0.47
1:F:398:LYS:C	1:F:400:TYR:N	2.73	0.47
1:E:7:PHE:CD2	1:F:85:GLU:OE1	2.68	0.46
1:F:405:ASP:OD1	1:F:405:ASP:N	2.40	0.46
1:A:100:VAL:HG13	1:A:228:GLU:HG3	1.96	0.46
1:B:397:TRP:C	1:B:399:ARG:N	2.73	0.46
1:D:180:TRP:HB3	1:D:181:PRO:HD3	1.96	0.46
1:F:20:PRO:HD2	1:F:21:GLU:OE2	2.14	0.46
1:F:395:LEU:O	1:F:397:TRP:CD1	2.69	0.46
1:A:324:LEU:HD23	5:A:1059:HOH:O	2.16	0.46
1:A:309:PRO:HG2	1:A:343:LYS:O	2.15	0.46
1:B:24:GLY:C	1:B:26:PRO:HD3	2.40	0.46
1:B:83:PRO:HG3	1:B:140:TYR:CZ	2.51	0.46
1:C:33:TYR:O	1:C:37:ARG:HB2	2.16	0.46
1:D:207:ASP:HB2	1:D:208:PRO:HD3	1.97	0.46
1:F:18:ARG:O	1:F:20:PRO:HD3	2.15	0.46
1:F:48:ASP:C	1:F:48:ASP:OD1	2.58	0.46
1:F:327:LYS:HA	1:F:332:PRO:CG	2.45	0.46
1:C:10:LEU:HG	1:D:99:TYR:CE2	2.50	0.46
1:D:324:LEU:CD2	1:D:328:LYS:HG3	2.45	0.46
1:F:284:LYS:O	1:F:285:VAL:C	2.57	0.46
1:B:237:ASP:OD1	1:B:240:GLU:HG3	2.16	0.46
1:F:206:LYS:CA	1:F:211:ASN:O	2.59	0.46
1:F:225:PRO:HA	1:F:226:PRO:HD3	1.79	0.46
1:F:330:PHE:O	1:F:332:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:THR:HA	1:F:283:LYS:O	2.16	0.46
1:A:112:VAL:O	1:A:116:VAL:HG23	2.15	0.46
1:D:371:LEU:HB2	1:D:412:MSE:HB3	1.97	0.46
1:C:71:LYS:HE3	1:C:173:ALA:HB1	1.97	0.46
1:D:186:ARG:HG2	1:D:380:ILE:HG21	1.98	0.46
1:E:311:ALA:HB2	1:E:342:PRO:HG3	1.91	0.46
1:F:44:LEU:O	1:F:45:ASP:C	2.59	0.46
1:F:112:VAL:HG22	3:F:950:ANP:O2A	2.16	0.46
1:F:212:VAL:CG1	1:F:214:TYR:HE1	2.28	0.46
1:B:250:ARG:NH1	1:B:252:TYR:HE1	2.04	0.46
1:C:161:VAL:CG1	1:C:162:GLU:N	2.78	0.46
1:D:86:VAL:N	1:D:87:PRO:CD	2.79	0.46
1:B:143:LYS:HB2	1:B:157:GLU:H	1.81	0.45
1:E:81:ILE:HD12	1:E:90:PHE:HE2	1.81	0.45
1:F:81:ILE:HD13	1:F:90:PHE:CE2	2.50	0.45
1:F:102:ARG:HB2	1:F:228:GLU:HA	1.98	0.45
1:F:254:ILE:CD1	1:F:285:VAL:HA	2.46	0.45
1:A:422:TYR:CE2	1:A:427:LYS:HD2	2.51	0.45
1:E:22:LEU:CD2	1:F:424:SER:HA	2.46	0.45
1:E:27:ASN:HB2	1:E:28:PRO:CD	2.46	0.45
1:F:58:ILE:CG2	1:F:74:VAL:HG22	2.46	0.45
1:B:64:ASP:CG	1:B:67:ARG:CG	2.89	0.45
1:C:71:LYS:CE	1:C:173:ALA:HB1	2.46	0.45
1:C:257:PHE:CG	1:C:285:VAL:HG11	2.51	0.45
1:D:230:LYS:HE2	1:D:260:ASN:O	2.16	0.45
1:E:295:ARG:O	1:E:299:THR:CG2	2.57	0.45
1:C:249:LYS:CE	1:C:249:LYS:CA	2.88	0.45
1:F:198:THR:CG2	1:F:203:PHE:HE1	2.30	0.45
1:C:127:ILE:O	1:C:127:ILE:HG13	2.16	0.45
1:D:45:ASP:O	1:D:49:VAL:HB	2.16	0.45
1:E:289:THR:O	1:E:292:GLU:N	2.49	0.45
1:F:45:ASP:OD2	1:F:104:THR:HB	2.16	0.45
1:F:64:ASP:CG	1:F:67:ARG:HB2	2.41	0.45
1:B:130:GLU:CG	1:B:141:THR:HG22	2.38	0.45
1:E:48:ASP:CG	1:E:105:ARG:HH22	2.23	0.45
1:F:43:SER:O	1:F:44:LEU:C	2.59	0.45
1:F:180:TRP:CZ2	1:F:184:LYS:HG3	2.50	0.45
1:F:254:ILE:HD13	1:F:285:VAL:HA	1.97	0.45
1:A:433:VAL:CG1	1:A:436:ILE:HD13	2.47	0.45
1:E:295:ARG:HG3	1:F:67:ARG:NH2	2.32	0.45
1:F:296:LEU:CD2	1:F:300:PHE:CZ	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:OD2	1:A:284:LYS:HD3	2.16	0.45
1:A:345:TYR:CD2	1:A:436:ILE:HD11	2.52	0.45
1:B:17:LYS:HD2	1:B:17:LYS:O	2.16	0.45
1:B:255:LYS:NZ	1:B:267:ASP:OD1	2.49	0.45
5:D:1032:HOH:O	1:E:221:LYS:HE3	2.17	0.45
1:E:232:HIS:O	1:E:347:GLY:HA2	2.17	0.45
1:E:358:PHE:CD2	1:E:358:PHE:C	2.95	0.45
1:B:255:LYS:CE	1:B:267:ASP:OD1	2.65	0.45
1:E:44:LEU:HB3	1:E:105:ARG:CZ	2.46	0.45
1:E:196:ILE:HD11	1:E:373:TYR:OH	2.17	0.45
1:F:37:ARG:HG2	1:F:41:GLU:OE2	2.16	0.45
1:A:102:ARG:HB2	1:A:228:GLU:HA	1.99	0.45
1:E:331:ASN:N	1:E:332:PRO:HD3	2.32	0.45
1:F:148:ILE:O	1:F:148:ILE:HG22	2.17	0.45
1:F:155:ILE:HG12	5:F:980:HOH:O	2.16	0.45
1:F:207:ASP:HB2	1:F:208:PRO:CD	2.43	0.45
1:B:248:LEU:HD22	1:B:252:TYR:HE2	1.79	0.44
1:C:87:PRO:HB3	1:C:155:ILE:HD11	1.99	0.44
1:E:280:LYS:HA	1:E:281:PRO:HD3	1.79	0.44
1:E:375:ASN:OD1	1:E:416:CYS:HA	2.17	0.44
1:F:105:ARG:HB3	1:F:377:ILE:HD11	1.98	0.44
1:F:392:VAL:HG22	1:F:444:LEU:HD11	1.98	0.44
1:A:102:ARG:HD3	1:A:104:THR:HG23	1.99	0.44
1:F:6:LYS:HE2	5:F:1026:HOH:O	2.17	0.44
1:F:33:TYR:CD2	1:F:33:TYR:C	2.94	0.44
1:F:83:PRO:HD3	1:F:133:PRO:HG3	1.99	0.44
1:A:137:LYS:H	1:A:137:LYS:CE	2.29	0.44
1:B:441:LYS:NZ	1:B:445:MSE:HE1	2.31	0.44
1:C:326:LEU:HD13	1:C:357:ALA:HB2	2.00	0.44
1:E:118:TYR:CE2	1:E:177:PRO:HD2	2.53	0.44
1:E:213:THR:CG2	1:E:215:TYR:OH	2.53	0.44
1:F:64:ASP:C	1:F:66:ALA:H	2.24	0.44
1:F:207:ASP:O	1:F:208:PRO:C	2.60	0.44
1:F:253:THR:H	1:F:256:GLU:HB2	1.83	0.44
1:A:96:SER:HB3	1:A:99:TYR:CE2	2.53	0.44
1:E:14:GLU:O	1:E:18:ARG:HG3	2.18	0.44
1:E:30:ARG:CG	5:E:1016:HOH:O	2.64	0.44
1:E:453:GLN:NE2	1:E:457:GLU:HG3	2.31	0.44
1:F:58:ILE:HG23	1:F:74:VAL:HG22	1.98	0.44
1:A:221:LYS:HD3	5:A:1047:HOH:O	2.17	0.44
1:A:319:GLU:O	1:A:323:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLU:CG	1:A:404:SER:N	2.73	0.44
1:B:64:ASP:CG	1:B:67:ARG:HG3	2.42	0.44
1:E:27:ASN:HB2	1:E:28:PRO:HD2	2.00	0.44
1:E:385:SER:HB3	1:F:385:SER:HB3	1.99	0.44
1:E:402:ILE:CG2	1:E:403:GLU:N	2.80	0.44
1:B:118:TYR:CE2	1:B:177:PRO:HD2	2.52	0.44
1:E:25:PHE:N	1:E:26:PRO:HD3	2.33	0.44
1:F:93:VAL:HG12	1:F:94:LEU:HG	1.99	0.44
1:A:18:ARG:O	1:B:419:LYS:HE3	2.17	0.44
1:A:108:TYR:CE2	1:A:427:LYS:HD3	2.53	0.44
1:C:121:MSE:HE2	1:D:237:ASP:OD2	2.18	0.44
1:C:423:LYS:NZ	1:D:382:ASP:OD1	2.50	0.44
1:D:161:VAL:CG1	1:D:162:GLU:N	2.81	0.44
1:F:35:THR:HG23	1:F:115:ALA:HB1	1.98	0.44
1:F:291:GLU:HG2	1:F:291:GLU:H	1.40	0.44
1:E:255:LYS:O	1:E:259:VAL:HG12	2.18	0.44
1:F:289:THR:HG22	1:F:292:GLU:CG	2.47	0.44
1:A:10:LEU:HD12	1:B:99:TYR:CZ	2.52	0.44
1:D:196:ILE:CD1	1:D:329:ILE:HD11	2.48	0.44
1:E:27:ASN:ND2	1:E:30:ARG:H	2.16	0.44
1:F:87:PRO:O	1:F:91:GLY:N	2.49	0.44
1:F:118:TYR:CE2	1:F:177:PRO:HD2	2.53	0.44
1:A:207:ASP:C	1:A:207:ASP:OD1	2.61	0.43
1:B:200:TYR:OH	1:B:376:LYS:NZ	2.51	0.43
1:C:144:LEU:HD12	1:C:144:LEU:O	2.17	0.43
1:C:207:ASP:CB	1:C:208:PRO:CD	2.88	0.43
1:F:12:PRO:O	1:F:16:PHE:HD2	2.01	0.43
1:A:207:ASP:CB	1:A:208:PRO:CD	2.94	0.43
1:B:237:ASP:CG	1:B:240:GLU:HG3	2.42	0.43
1:B:255:LYS:O	1:B:259:VAL:HG13	2.19	0.43
1:C:254:ILE:CG2	1:C:274:LEU:HD21	2.48	0.43
1:D:404:SER:C	1:D:406:GLN:N	2.76	0.43
1:A:96:SER:HB2	1:A:109:GLY:HA2	2.00	0.43
1:A:306:PHE:HB2	5:A:932:HOH:O	2.18	0.43
1:C:338:ILE:HG22	1:C:447:VAL:HG13	2.00	0.43
1:D:207:ASP:CB	1:D:208:PRO:CD	2.94	0.43
1:F:53:LEU:HD11	1:F:220:ASN:OD1	2.18	0.43
1:F:127:ILE:CD1	1:F:174:ILE:HD11	2.48	0.43
1:A:454:TYR:CD2	1:A:454:TYR:C	2.96	0.43
1:C:48:ASP:OD1	1:C:105:ARG:NH2	2.49	0.43
1:E:397:TRP:C	1:E:399:ARG:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ILE:HD12	1:F:203:PHE:HE2	1.83	0.43
1:F:93:VAL:O	1:F:94:LEU:HB2	2.18	0.43
1:F:127:ILE:HD12	1:F:174:ILE:HD11	1.97	0.43
1:F:207:ASP:OD1	1:F:211:ASN:HB2	2.18	0.43
1:F:386:ASP:OD1	1:F:387:VAL:N	2.51	0.43
1:A:147:ASP:OD1	1:A:147:ASP:C	2.60	0.43
1:C:148:ILE:HG13	1:C:149:ASN:N	2.34	0.43
1:C:318:GLY:O	1:C:322:ILE:HG13	2.18	0.43
1:E:60:ILE:HG22	1:E:208:PRO:HG3	2.00	0.43
1:F:179:ASP:OD1	1:F:179:ASP:C	2.61	0.43
1:F:180:TRP:CD2	1:F:208:PRO:CG	2.91	0.43
1:F:250:ARG:CB	5:F:1023:HOH:O	2.66	0.43
1:A:323:GLU:OE2	5:A:948:HOH:O	2.21	0.43
1:B:21:GLU:HG3	1:B:26:PRO:HA	2.00	0.43
1:C:29:ALA:HB2	1:C:179:ASP:HB3	2.01	0.43
1:D:157:GLU:HG3	5:D:1002:HOH:O	2.17	0.43
1:B:49:VAL:O	1:B:49:VAL:HG12	2.19	0.43
1:C:96:SER:HB2	1:C:109:GLY:CA	2.48	0.43
1:D:93:VAL:O	1:D:94:LEU:HB2	2.19	0.43
1:F:319:GLU:HA	1:F:337:SER:OG	2.19	0.43
1:A:25:PHE:N	1:A:26:PRO:HD3	2.33	0.43
1:B:157:GLU:HG2	5:B:1038:HOH:O	2.17	0.43
1:C:123:GLN:NE2	1:C:175:SER:HB2	2.34	0.43
1:C:358:PHE:CD2	1:C:358:PHE:C	2.96	0.43
1:D:116:VAL:CG2	1:D:127:ILE:HD13	2.49	0.43
1:D:179:ASP:OD1	1:D:179:ASP:C	2.62	0.43
1:F:37:ARG:HD2	5:F:983:HOH:O	2.18	0.43
1:A:289:THR:O	1:A:290:GLU:C	2.62	0.42
1:B:6:LYS:CE	5:B:1051:HOH:O	2.66	0.42
1:B:253:THR:HB	1:B:281:PRO:O	2.18	0.42
1:D:227:GLN:NE2	5:D:965:HOH:O	2.52	0.42
1:F:19:ASN:CB	1:F:22:LEU:HD22	2.48	0.42
1:A:34:GLN:NE2	1:A:37:ARG:NH1	2.67	0.42
1:D:117:LEU:C	1:D:121:MSE:HE3	2.44	0.42
1:E:387:VAL:HG12	1:E:430:ILE:HB	2.01	0.42
1:F:289:THR:CG2	1:F:292:GLU:CG	2.96	0.42
1:A:224:LYS:HA	1:A:225:PRO:HD3	1.95	0.42
1:B:224:LYS:HA	1:B:225:PRO:HD3	1.88	0.42
1:B:253:THR:HA	1:B:283:LYS:O	2.18	0.42
1:B:397:TRP:HB3	1:B:402:ILE:HD12	2.00	0.42
1:F:129:ILE:HD12	1:F:144:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:ASN:HD22	1:F:331:ASN:HA	1.52	0.42
1:F:388:ILE:O	1:F:392:VAL:HG23	2.20	0.42
1:E:311:ALA:CB	1:E:342:PRO:HG2	2.43	0.42
1:C:304:GLU:OE2	1:E:307:ARG:NH2	2.53	0.42
1:F:34:GLN:NE2	1:F:38:GLU:OE1	2.49	0.42
1:F:127:ILE:CG1	1:F:174:ILE:HD13	2.50	0.42
1:A:27:ASN:HD21	1:A:30:ARG:H	1.62	0.42
1:A:32:LEU:HA	1:A:176:ILE:HD11	2.01	0.42
1:B:229:VAL:HG11	1:B:313:SER:HB3	2.01	0.42
1:B:368:PRO:HB3	1:B:409:MSE:HE3	2.00	0.42
1:F:57:LYS:HD3	1:F:204:ILE:HD12	2.00	0.42
1:A:64:ASP:O	1:A:68:GLN:N	2.52	0.42
1:A:146:ILE:HG22	1:A:148:ILE:HD13	2.02	0.42
1:B:21:GLU:CD	1:B:21:GLU:H	2.28	0.42
1:C:247:ASN:N	1:C:247:ASN:HD22	2.16	0.42
1:D:434:GLU:CD	5:D:1007:HOH:O	2.63	0.42
1:E:67:ARG:HG2	1:F:298:GLU:OE1	2.20	0.42
1:E:273:ILE:HD11	1:E:306:PHE:CZ	2.55	0.42
1:E:402:ILE:HG22	1:E:403:GLU:N	2.33	0.42
1:F:33:TYR:OH	1:F:380:ILE:CG1	2.66	0.42
1:A:117:LEU:CD2	1:A:148:ILE:HD12	2.50	0.42
1:C:120:GLN:NE2	1:C:146:ILE:N	2.56	0.42
1:C:460:LYS:NZ	5:C:930:HOH:O	2.51	0.42
1:F:358:PHE:CD2	1:F:358:PHE:C	2.97	0.42
1:C:53:LEU:HA	1:C:54:PRO:HD3	1.86	0.42
1:C:206:LYS:HA	1:C:211:ASN:O	2.19	0.42
1:C:356:VAL:O	1:C:356:VAL:HG13	2.19	0.42
1:E:310:SER:C	1:E:312:ASP:H	2.28	0.42
1:F:92:ARG:O	1:F:113:LYS:CE	2.55	0.42
1:B:343:LYS:HE2	5:B:1020:HOH:O	2.19	0.42
1:C:332:PRO:HD2	5:C:1026:HOH:O	2.20	0.42
1:C:438:LYS:HE2	5:C:959:HOH:O	2.19	0.42
1:E:27:ASN:HD22	1:E:29:ALA:H	1.68	0.42
1:E:193:ARG:HH11	1:E:193:ARG:HD2	1.71	0.42
1:A:423:LYS:HG2	1:A:431:ALA:CA	2.50	0.41
1:E:37:ARG:HG3	1:E:41:GLU:OE2	2.20	0.41
1:F:63:ILE:HD11	1:F:71:LYS:HD2	2.02	0.41
1:F:233:PRO:HG3	1:F:265:ILE:CD1	2.50	0.41
1:F:307:ARG:NH2	5:F:1031:HOH:O	2.52	0.41
1:A:100:VAL:HG13	1:A:228:GLU:CG	2.50	0.41
1:B:318:GLY:O	1:B:322:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:PHE:C	1:D:8:THR:CG2	2.93	0.41
1:F:117:LEU:HD23	1:F:148:ILE:CD1	2.45	0.41
1:F:320:ASP:OD1	1:F:321:LEU:HG	2.20	0.41
1:A:251:ASP:O	1:A:251:ASP:CG	2.62	0.41
1:B:133:PRO:O	1:B:135:ASN:N	2.53	0.41
1:E:19:ASN:N	1:E:20:PRO:HD3	2.36	0.41
1:D:96:SER:HB2	1:D:109:GLY:HA2	2.02	0.41
1:E:99:TYR:CE2	1:F:10:LEU:HG	2.55	0.41
1:A:195:TYR:OH	1:A:216:PRO:O	2.33	0.41
1:C:25:PHE:N	1:C:26:PRO:CD	2.83	0.41
1:E:277:ALA:CB	1:E:299:THR:HG21	2.48	0.41
1:A:374:ALA:HA	1:A:415:LEU:O	2.20	0.41
1:B:441:LYS:NZ	1:B:445:MSE:CE	2.83	0.41
1:E:22:LEU:HD22	1:F:424:SER:HA	2.01	0.41
1:F:30:ARG:NH2	1:F:34:GLN:OE1	2.52	0.41
1:A:222:ILE:HA	1:A:223:PRO:HD3	1.93	0.41
1:B:167:PHE:CA	5:B:1050:HOH:O	2.67	0.41
1:C:48:ASP:CG	1:C:105:ARG:HH22	2.29	0.41
1:D:312:ASP:OD1	1:D:312:ASP:N	2.51	0.41
1:F:107:MSE:HE2	1:F:108:TYR:CE1	2.56	0.41
1:F:152:GLU:HA	1:F:153:PRO:HD3	1.86	0.41
1:F:404:SER:OG	1:F:406:GLN:O	2.29	0.41
1:A:237:ASP:OD2	1:B:17:LYS:NZ	2.53	0.41
1:A:238:ARG:NH1	1:A:290:GLU:O	2.53	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.94	0.41
1:C:330:PHE:CA	5:C:945:HOH:O	2.62	0.41
1:F:72:VAL:O	1:F:173:ALA:HA	2.21	0.41
1:F:212:VAL:CG1	1:F:214:TYR:CE1	3.04	0.41
1:A:145:LYS:NZ	1:B:290:GLU:HG3	2.36	0.41
1:A:237:ASP:OD2	1:B:121:MSE:HE3	2.21	0.41
1:A:273:ILE:HD11	1:A:306:PHE:HE1	1.85	0.41
1:A:389:TRP:CE3	5:A:1058:HOH:O	2.74	0.41
1:B:232:HIS:CD2	1:B:309:PRO:HG3	2.56	0.41
1:E:112:VAL:HG12	3:E:940:ANP:O2A	2.21	0.41
1:E:224:LYS:HA	1:E:225:PRO:HD3	1.87	0.41
1:F:4:LYS:N	5:F:974:HOH:O	2.53	0.41
1:F:55:ASN:HA	1:F:202:GLU:HB3	2.02	0.41
1:F:187:ILE:O	1:F:191:ILE:HG12	2.21	0.41
1:F:345:TYR:O	1:F:346:GLN:C	2.64	0.41
1:F:420:ILE:HA	1:F:421:PRO:HD3	1.92	0.41
1:C:9:SER:HB3	1:D:95:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ILE:HD11	1:D:329:ILE:HD11	2.03	0.41
1:D:232:HIS:CG	1:D:233:PRO:HD2	2.56	0.41
1:E:266:GLY:O	1:E:267:ASP:C	2.64	0.41
1:F:34:GLN:O	1:F:38:GLU:CG	2.67	0.41
1:F:80:GLY:C	1:F:81:ILE:HG13	2.46	0.41
1:F:245:ILE:C	1:F:247:ASN:N	2.79	0.41
1:F:374:ALA:O	1:F:375:ASN:C	2.61	0.41
1:F:424:SER:O	1:F:427:LYS:HA	2.20	0.41
1:B:196:ILE:HD12	1:B:196:ILE:HA	1.83	0.40
1:C:12:PRO:HG3	1:D:12:PRO:HG3	2.03	0.40
1:F:236:VAL:O	1:F:236:VAL:HG13	2.21	0.40
1:C:291:GLU:H	1:C:291:GLU:CD	2.29	0.40
1:D:335:ALA:HA	1:D:356:VAL:O	2.22	0.40
1:D:407:TYR:CD1	1:D:409:MSE:HE2	2.56	0.40
1:D:420:ILE:HA	1:D:421:PRO:HD3	1.88	0.40
1:E:134:VAL:HB	5:E:1049:HOH:O	2.21	0.40
1:F:55:ASN:HB2	1:F:77:ASN:CG	2.47	0.40
1:F:340:ARG:HH11	1:F:439:GLU:CD	2.30	0.40
1:C:192:LYS:HE3	5:C:970:HOH:O	2.20	0.40
1:D:226:PRO:HG3	1:D:315:SER:HB2	2.02	0.40
1:E:17:LYS:HD3	1:E:17:LYS:C	2.46	0.40
1:E:225:PRO:HA	1:E:226:PRO:HD3	1.92	0.40
1:F:180:TRP:CB	1:F:208:PRO:HG2	2.48	0.40
1:F:256:GLU:O	1:F:260:ASN:HB2	2.21	0.40
1:F:381:TYR:N	1:F:428:GLU:OE1	2.46	0.40
1:A:284:LYS:CD	1:A:286:LYS:HE2	2.50	0.40
1:C:239:GLU:CG	5:C:936:HOH:O	2.68	0.40
1:C:411:VAL:HG13	1:C:444:LEU:HD21	2.03	0.40
1:D:21:GLU:CD	1:D:21:GLU:N	2.75	0.40
1:D:438:LYS:HE3	1:D:438:LYS:HB2	1.84	0.40
1:E:461:GLU:C	5:E:1058:HOH:O	2.64	0.40
1:F:53:LEU:HG	1:F:222:ILE:HD11	2.02	0.40
1:B:453:GLN:HE21	1:B:457:GLU:CD	2.30	0.40
1:D:222:ILE:HG13	1:D:223:PRO:HD2	2.03	0.40
1:E:80:GLY:HA2	1:E:170:THR:OG1	2.22	0.40
1:E:207:ASP:HB2	1:E:208:PRO:HD2	2.03	0.40
1:E:236:VAL:O	1:E:297:VAL:HG13	2.21	0.40
1:E:238:ARG:HG2	1:E:297:VAL:HG21	2.03	0.40
1:E:368:PRO:HD3	1:E:407:TYR:CE2	2.56	0.40
1:F:47:THR:HG21	1:F:54:PRO:HA	2.04	0.40
1:F:117:LEU:CD2	1:F:148:ILE:HD11	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:LEU:CD2	1:F:300:PHE:CE2	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/472 (97%)	440 (96%)	17 (4%)	0	100	100
1	B	453/472 (96%)	426 (94%)	24 (5%)	3 (1%)	18	23
1	C	464/472 (98%)	448 (97%)	15 (3%)	1 (0%)	43	55
1	D	459/472 (97%)	440 (96%)	19 (4%)	0	100	100
1	E	452/472 (96%)	427 (94%)	22 (5%)	3 (1%)	18	23
1	F	444/472 (94%)	379 (85%)	48 (11%)	17 (4%)	2	1
All	All	2729/2832 (96%)	2560 (94%)	145 (5%)	24 (1%)	14	17

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	208	PRO
1	F	245	ILE
1	F	246	ASN
1	F	332	PRO
1	F	399	ARG
1	C	166	GLY
1	E	290	GLU
1	F	26	PRO
1	F	63	ILE
1	F	148	ILE
1	F	340	ARG

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Mol	Chain	Res	Type
1	B	166	GLY
1	E	247	ASN
1	F	65	ASP
1	B	134	VAL
1	F	94	LEU
1	F	126	PRO
1	F	398	LYS
1	E	398	LYS
1	F	46	ALA
1	F	87	PRO
1	F	101	ASN
1	B	156	VAL
1	F	125	LYS

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	407/412 (99%)	377 (93%)	30 (7%)	13	17
1	B	402/412 (98%)	378 (94%)	24 (6%)	17	25
1	C	410/412 (100%)	384 (94%)	26 (6%)	16	23
1	D	404/412 (98%)	379 (94%)	25 (6%)	16	24
1	E	407/412 (99%)	370 (91%)	37 (9%)	9	11
1	F	389/412 (94%)	337 (87%)	52 (13%)	4	4
All	All	2419/2472 (98%)	2225 (92%)	194 (8%)	11	15

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	22	LEU
1	A	27	ASN
1	A	62	LEU
1	A	81	ILE

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Mol	Chain	Res	Type
1	A	100	VAL
1	A	110	LEU
1	A	128	GLU
1	A	137	LYS
1	A	160	SER
1	A	194	THR
1	A	196	ILE
1	A	224	LYS
1	A	238	ARG
1	A	242	LYS
1	A	249	LYS
1	A	259	VAL
1	A	268	THR
1	A	285	VAL
1	A	296	LEU
1	A	321	LEU
1	A	364	VAL
1	A	371	LEU
1	A	380	ILE
1	A	395	LEU
1	A	405	ASP
1	A	409	MSE
1	A	427	LYS
1	A	434	GLU
1	A	456	SER
1	B	6	LYS
1	B	17	LYS
1	B	22	LEU
1	B	62	LEU
1	B	65	ASP
1	B	67	ARG
1	B	137	LYS
1	B	144	LEU
1	B	148	ILE
1	B	157	GLU
1	B	158	ARG
1	B	174	ILE
1	B	185	SER
1	B	198	THR
1	B	247	ASN
1	B	285	VAL
1	B	290	GLU

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Mol	Chain	Res	Type
1	B	296	LEU
1	B	304	GLU
1	B	321	LEU
1	B	324	LEU
1	B	340	ARG
1	B	371	LEU
1	B	444	LEU
1	C	17	LYS
1	C	22	LEU
1	C	30	ARG
1	C	62	LEU
1	C	100	VAL
1	C	110	LEU
1	C	113	LYS
1	C	138	ARG
1	C	144	LEU
1	C	152	GLU
1	C	196	ILE
1	C	221	LYS
1	C	239	GLU
1	C	244	LEU
1	C	249	LYS
1	C	259	VAL
1	C	263	GLN
1	C	267	ASP
1	C	285	VAL
1	C	290	GLU
1	C	296	LEU
1	C	321	LEU
1	C	371	LEU
1	C	395	LEU
1	C	402	ILE
1	C	460	LYS
1	D	17	LYS
1	D	22	LEU
1	D	30	ARG
1	D	62	LEU
1	D	85	GLU
1	D	148	ILE
1	D	174	ILE
1	D	186	ARG
1	D	250	ARG

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Mol	Chain	Res	Type
1	D	268	THR
1	D	276	LEU
1	D	285	VAL
1	D	291	GLU
1	D	296	LEU
1	D	304	GLU
1	D	312	ASP
1	D	321	LEU
1	D	324	LEU
1	D	338	ILE
1	D	340	ARG
1	D	371	LEU
1	D	385	SER
1	D	418	THR
1	D	444	LEU
1	D	458	LYS
1	E	6	LYS
1	E	17	LYS
1	E	37	ARG
1	E	62	LEU
1	E	85	GLU
1	E	100	VAL
1	E	107	MSE
1	E	110	LEU
1	E	113	LYS
1	E	134	VAL
1	E	138	ARG
1	E	161	VAL
1	E	174	ILE
1	E	196	ILE
1	E	213	THR
1	E	217	ARG
1	E	222	ILE
1	E	240	GLU
1	E	241	ILE
1	E	259	VAL
1	E	273	ILE
1	E	285	VAL
1	E	289	THR
1	E	296	LEU
1	E	298	GLU
1	E	299	THR

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Mol	Chain	Res	Type
1	E	310	SER
1	E	312	ASP
1	E	313	SER
1	E	321	LEU
1	E	338	ILE
1	E	340	ARG
1	E	371	LEU
1	E	398	LYS
1	E	404	SER
1	E	424	SER
1	E	447	VAL
1	F	17	LYS
1	F	21	GLU
1	F	22	LEU
1	F	30	ARG
1	F	47	THR
1	F	57	LYS
1	F	62	LEU
1	F	63	ILE
1	F	77	ASN
1	F	79	ILE
1	F	84	GLN
1	F	110	LEU
1	F	112	VAL
1	F	119	SER
1	F	120	GLN
1	F	124	ASP
1	F	127	ILE
1	F	131	THR
1	F	134	VAL
1	F	139	ILE
1	F	150	LYS
1	F	172	VAL
1	F	174	ILE
1	F	175	SER
1	F	196	ILE
1	F	198	THR
1	F	208	PRO
1	F	218	LEU
1	F	219	THR
1	F	220	ASN
1	F	238	ARG

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Mol	Chain	Res	Type
1	F	244	LEU
1	F	251	ASP
1	F	253	THR
1	F	259	VAL
1	F	285	VAL
1	F	289	THR
1	F	290	GLU
1	F	291	GLU
1	F	298	GLU
1	F	307	ARG
1	F	312	ASP
1	F	315	SER
1	F	331	ASN
1	F	361	SER
1	F	371	LEU
1	F	382	ASP
1	F	390	LYS
1	F	395	LEU
1	F	405	ASP
1	F	427	LYS
1	F	430	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	27	ASN
1	A	73	ASN
1	A	101	ASN
1	A	120	GLN
1	A	123	GLN
1	A	247	ASN
1	B	120	GLN
1	B	122	HIS
1	B	453	GLN
1	C	19	ASN
1	C	68	GLN
1	C	101	ASN
1	C	120	GLN
1	C	123	GLN
1	C	247	ASN
1	C	348	HIS

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Mol	Chain	Res	Type
1	C	453	GLN
1	D	247	ASN
1	D	346	GLN
1	E	19	ASN
1	E	27	ASN
1	E	88	ASN
1	E	120	GLN
1	E	282	ASN
1	E	408	GLN
1	E	453	GLN
1	F	73	ASN
1	F	77	ASN
1	F	120	GLN
1	F	220	ASN
1	F	227	GLN
1	F	331	ASN
1	F	453	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 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
3	ANP	C	920	2	33,33,33	2.42	12 (36%)	45,52,52	1.86	10 (22%)
3	ANP	F	950	2	33,33,33	2.45	13 (39%)	45,52,52	2.07	12 (26%)
3	ANP	E	940	2	33,33,33	2.35	13 (39%)	45,52,52	1.63	10 (22%)
3	ANP	A	900	2	33,33,33	2.25	10 (30%)	45,52,52	1.54	10 (22%)
3	ANP	B	910	2	33,33,33	2.30	11 (33%)	45,52,52	2.06	11 (24%)
3	ANP	D	930	2	33,33,33	2.42	12 (36%)	45,52,52	1.82	11 (24%)

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
3	ANP	C	920	2	-	4/18/38/38	0/3/3/3
3	ANP	F	950	2	-	4/18/38/38	0/3/3/3
3	ANP	E	940	2	-	3/18/38/38	0/3/3/3
3	ANP	A	900	2	-	4/18/38/38	0/3/3/3
3	ANP	B	910	2	-	4/18/38/38	0/3/3/3
3	ANP	D	930	2	-	4/18/38/38	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	920	ANP	PB-O3A	-7.83	1.49	1.59
3	F	950	ANP	PA-O3A	-7.75	1.51	1.59
3	D	930	ANP	PA-O3A	-7.06	1.51	1.59
3	C	920	ANP	PA-O3A	-6.70	1.52	1.59
3	A	900	ANP	PA-O3A	-6.67	1.52	1.59
3	E	940	ANP	PA-O3A	-6.42	1.52	1.59
3	F	950	ANP	PB-O3A	-6.34	1.51	1.59
3	D	930	ANP	PB-O3A	-6.25	1.51	1.59
3	B	910	ANP	PB-O3A	-5.91	1.51	1.59
3	B	910	ANP	PA-O3A	-5.85	1.53	1.59
3	A	900	ANP	PB-O3A	-5.37	1.52	1.59
3	E	940	ANP	PB-O3A	-5.21	1.52	1.59
3	F	950	ANP	C5-C4	4.87	1.47	1.39
3	A	900	ANP	C5-C4	4.44	1.47	1.39
3	E	940	ANP	C5-C4	4.35	1.46	1.39
3	C	920	ANP	C5-C4	4.12	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	930	ANP	C5-C4	4.12	1.46	1.39
3	B	910	ANP	C5-N7	-4.04	1.31	1.39
3	E	940	ANP	C5-N7	-3.68	1.32	1.39
3	B	910	ANP	PG-O2G	-3.53	1.47	1.56
3	E	940	ANP	PG-O1G	3.32	1.51	1.46
3	B	910	ANP	C8-N9	-3.31	1.31	1.37
3	D	930	ANP	PG-O2G	-3.30	1.48	1.56
3	F	950	ANP	C5-N7	-3.21	1.33	1.39
3	B	910	ANP	PB-O2B	-3.19	1.48	1.56
3	A	900	ANP	PG-O2G	-3.18	1.48	1.56
3	D	930	ANP	C5-N7	-3.16	1.33	1.39
3	E	940	ANP	PG-O3G	-3.12	1.48	1.56
3	C	920	ANP	C5-N7	-3.09	1.33	1.39
3	A	900	ANP	PB-O2B	-3.05	1.48	1.56
3	D	930	ANP	PG-O1G	3.03	1.50	1.46
3	D	930	ANP	PB-O1B	2.92	1.50	1.46
3	C	920	ANP	PB-O2B	-2.92	1.49	1.56
3	E	940	ANP	PG-O2G	-2.89	1.49	1.56
3	E	940	ANP	C4-N9	-2.85	1.31	1.37
3	D	930	ANP	C5-C6	2.84	1.48	1.41
3	B	910	ANP	C5-C4	2.82	1.44	1.39
3	E	940	ANP	PB-O2B	-2.77	1.49	1.56
3	C	920	ANP	C5-C6	2.75	1.48	1.41
3	A	900	ANP	C5-N7	-2.72	1.34	1.39
3	B	910	ANP	PG-O3G	-2.71	1.49	1.56
3	A	900	ANP	PG-O3G	-2.68	1.49	1.56
3	C	920	ANP	PG-O2G	-2.65	1.49	1.56
3	F	950	ANP	C5-C6	2.63	1.48	1.41
3	A	900	ANP	C4-N9	-2.63	1.32	1.37
3	B	910	ANP	PB-O1B	2.56	1.50	1.46
3	E	940	ANP	C5-C6	2.53	1.48	1.41
3	B	910	ANP	PG-O1G	2.53	1.50	1.46
3	F	950	ANP	C6-N6	2.50	1.40	1.34
3	F	950	ANP	PG-O3G	-2.50	1.50	1.56
3	F	950	ANP	PG-O2G	-2.48	1.50	1.56
3	D	930	ANP	PB-O2B	-2.44	1.50	1.56
3	D	930	ANP	PA-O5'	-2.44	1.49	1.59
3	E	940	ANP	PB-O1B	2.42	1.49	1.46
3	F	950	ANP	PA-O5'	-2.38	1.50	1.59
3	D	930	ANP	C6-N6	2.36	1.40	1.34
3	F	950	ANP	C8-N7	2.30	1.36	1.31
3	A	900	ANP	PG-O1G	2.28	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	930	ANP	C4-N9	-2.28	1.33	1.37
3	A	900	ANP	C5-C6	2.24	1.47	1.41
3	F	950	ANP	PG-O1G	2.23	1.49	1.46
3	C	920	ANP	PG-O3G	-2.15	1.51	1.56
3	F	950	ANP	PB-O1B	2.14	1.49	1.46
3	F	950	ANP	PB-O2B	-2.14	1.51	1.56
3	C	920	ANP	PB-O1B	2.12	1.49	1.46
3	E	940	ANP	PA-O5'	-2.11	1.51	1.59
3	C	920	ANP	PA-O5'	-2.07	1.51	1.59
3	C	920	ANP	C8-N7	2.06	1.35	1.31
3	C	920	ANP	PG-O1G	2.06	1.49	1.46
3	E	940	ANP	C8-N9	-2.04	1.34	1.37
3	B	910	ANP	PA-O5'	-2.02	1.51	1.59

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	910	ANP	C5-C4-N3	-6.16	118.23	126.72
3	F	950	ANP	C5-C4-N3	-6.02	118.43	126.72
3	C	920	ANP	C5-C4-N3	-5.71	118.86	126.72
3	D	930	ANP	C5-C4-N3	-5.38	119.31	126.72
3	E	940	ANP	C5-C4-N3	-5.02	119.81	126.72
3	F	950	ANP	N3-C4-N9	4.91	135.52	127.17
3	B	910	ANP	N3-C4-N9	4.67	135.12	127.17
3	C	920	ANP	N3-C4-N9	4.63	135.04	127.17
3	B	910	ANP	C4-C5-N7	-4.52	105.42	110.58
3	F	950	ANP	O1G-PG-N3B	-4.49	105.16	111.77
3	F	950	ANP	O4'-C1'-N9	4.27	116.28	108.09
3	A	900	ANP	C5-C4-N3	-4.13	121.04	126.72
3	B	910	ANP	C5-N7-C8	4.08	109.87	103.45
3	D	930	ANP	C4-C5-N7	-4.08	105.92	110.58
3	D	930	ANP	N3-C4-N9	4.03	134.03	127.17
3	C	920	ANP	C2-N3-C4	3.78	121.07	111.83
3	E	940	ANP	N3-C4-N9	3.74	133.52	127.17
3	A	900	ANP	N3-C4-N9	3.60	133.29	127.17
3	E	940	ANP	C4-C5-N7	-3.59	106.48	110.58
3	B	910	ANP	N9-C8-N7	-3.51	108.95	113.94
3	D	930	ANP	C2-N3-C4	3.49	120.36	111.83
3	C	920	ANP	N3-C2-N1	-3.44	123.37	128.58
3	F	950	ANP	C2-N3-C4	3.42	120.19	111.83
3	F	950	ANP	C3'-C2'-C1'	3.42	107.93	101.46
3	D	930	ANP	C5-N7-C8	3.39	108.77	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	910	ANP	C2-N3-C4	3.38	120.10	111.83
3	C	920	ANP	O1G-PG-N3B	-3.27	106.96	111.77
3	E	940	ANP	C2-N3-C4	3.24	119.73	111.83
3	A	900	ANP	N3-C2-N1	-3.22	123.71	128.58
3	B	910	ANP	C4-N9-C8	3.21	109.11	105.74
3	F	950	ANP	C4-C5-N7	-3.20	106.92	110.58
3	C	920	ANP	C4-C5-N7	-3.18	106.95	110.58
3	D	930	ANP	N3-C2-N1	-3.17	123.78	128.58
3	C	920	ANP	C5-N7-C8	3.00	108.17	103.45
3	B	910	ANP	N3-C2-N1	-2.99	124.06	128.58
3	A	900	ANP	C2-N3-C4	2.95	119.05	111.83
3	A	900	ANP	C4-N9-C8	2.85	108.73	105.74
3	F	950	ANP	N3-C2-N1	-2.80	124.35	128.58
3	D	930	ANP	C4-N9-C8	2.78	108.65	105.74
3	D	930	ANP	N9-C8-N7	-2.77	110.00	113.94
3	E	940	ANP	N3-C2-N1	-2.72	124.46	128.58
3	A	900	ANP	C4-C5-N7	-2.65	107.55	110.58
3	E	940	ANP	C5-N7-C8	2.59	107.53	103.45
3	C	920	ANP	C4-N9-C8	2.58	108.45	105.74
3	F	950	ANP	C5-N7-C8	2.58	107.50	103.45
3	C	920	ANP	N9-C8-N7	-2.54	110.33	113.94
3	D	930	ANP	O1G-PG-N3B	-2.48	108.12	111.77
3	A	900	ANP	C2-N1-C6	2.39	122.66	118.73
3	D	930	ANP	C6-C5-N7	2.31	136.54	132.09
3	F	950	ANP	C4'-O4'-C1'	2.26	114.45	109.47
3	E	940	ANP	C6-C5-N7	2.24	136.41	132.09
3	B	910	ANP	C4'-O4'-C1'	2.15	114.21	109.47
3	E	940	ANP	C4-N9-C8	2.15	107.99	105.74
3	A	900	ANP	C6-C5-N7	2.14	136.22	132.09
3	A	900	ANP	C5-N7-C8	2.14	106.81	103.45
3	F	950	ANP	C2'-C1'-N9	-2.11	108.06	113.30
3	B	910	ANP	C3'-C2'-C1'	2.11	105.45	101.46
3	E	940	ANP	O2B-PB-O3A	2.11	111.68	104.64
3	B	910	ANP	N6-C6-N1	2.10	123.06	118.38
3	D	930	ANP	C2-N1-C6	2.08	122.15	118.73
3	C	920	ANP	C6-C5-N7	2.08	136.10	132.09
3	A	900	ANP	O2B-PB-O3A	2.06	111.52	104.64
3	F	950	ANP	C2-N1-C6	2.04	122.08	118.73
3	E	940	ANP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	ANP	PB-N3B-PG-O1G
3	A	900	ANP	PG-N3B-PB-O1B
3	A	900	ANP	PA-O3A-PB-O1B
3	B	910	ANP	PB-N3B-PG-O1G
3	B	910	ANP	PG-N3B-PB-O1B
3	B	910	ANP	PA-O3A-PB-O2B
3	C	920	ANP	PB-N3B-PG-O1G
3	C	920	ANP	PG-N3B-PB-O1B
3	C	920	ANP	PA-O3A-PB-O1B
3	D	930	ANP	PB-N3B-PG-O1G
3	D	930	ANP	PG-N3B-PB-O1B
3	D	930	ANP	PA-O3A-PB-O2B
3	E	940	ANP	PB-N3B-PG-O1G
3	E	940	ANP	PG-N3B-PB-O1B
3	E	940	ANP	PA-O3A-PB-O1B
3	F	950	ANP	PB-N3B-PG-O1G
3	F	950	ANP	PG-N3B-PB-O1B
3	F	950	ANP	PA-O3A-PB-O2B
3	A	900	ANP	PA-O3A-PB-O2B
3	C	920	ANP	PA-O3A-PB-O2B
3	B	910	ANP	PA-O3A-PB-O1B
3	D	930	ANP	PA-O3A-PB-O1B
3	F	950	ANP	PA-O3A-PB-O1B

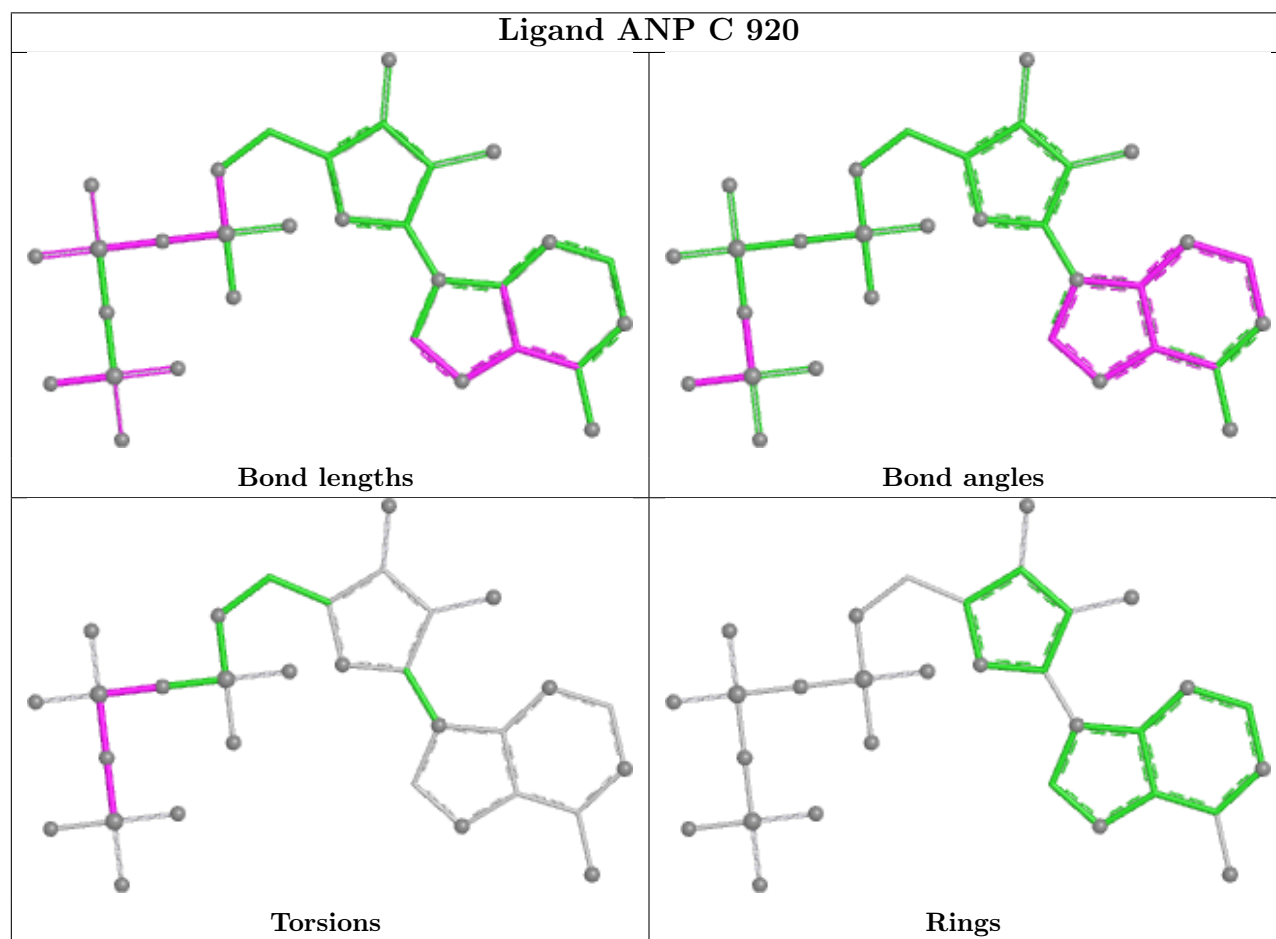
There are no ring outliers.

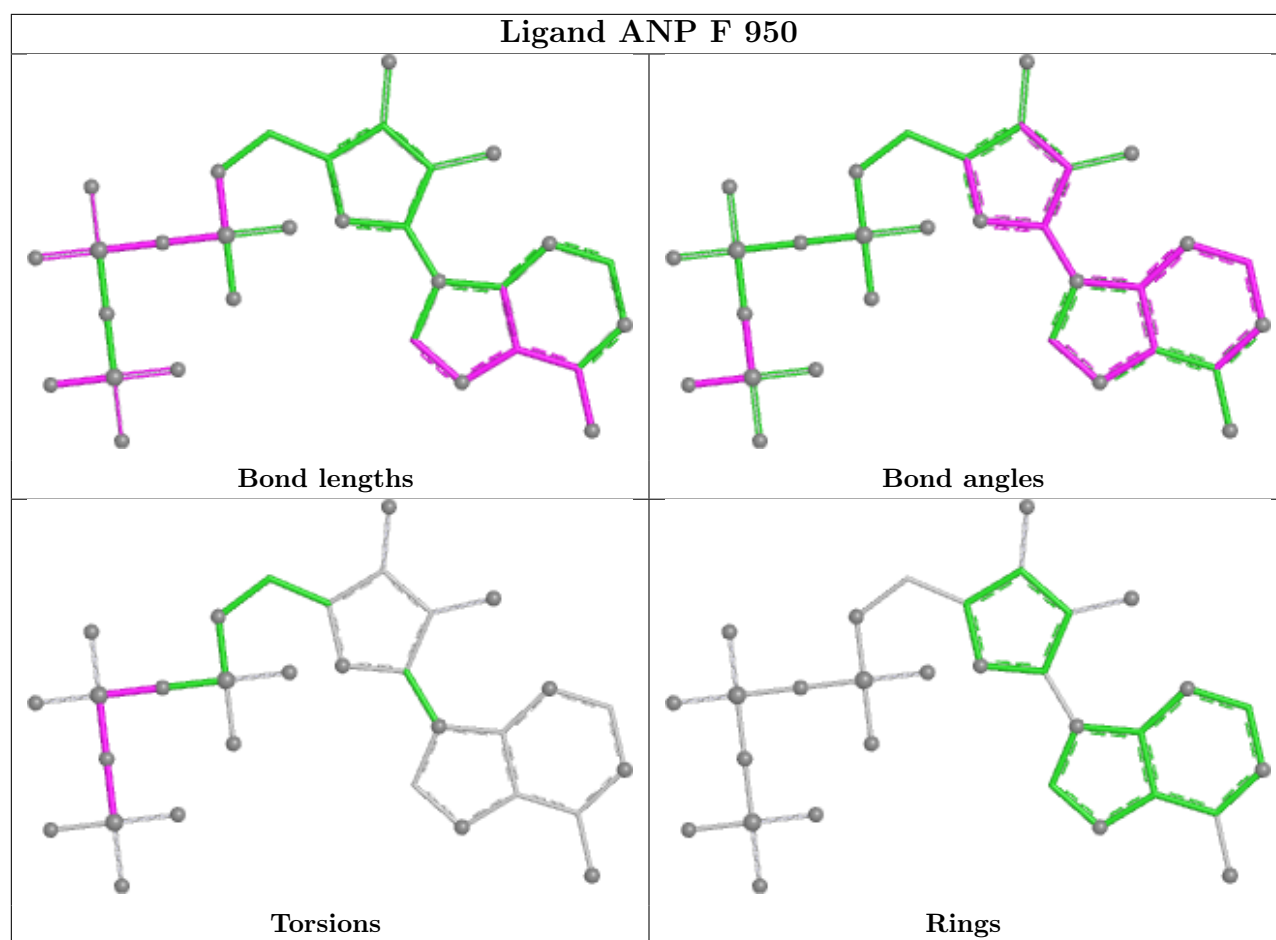
4 monomers are involved in 8 short contacts:

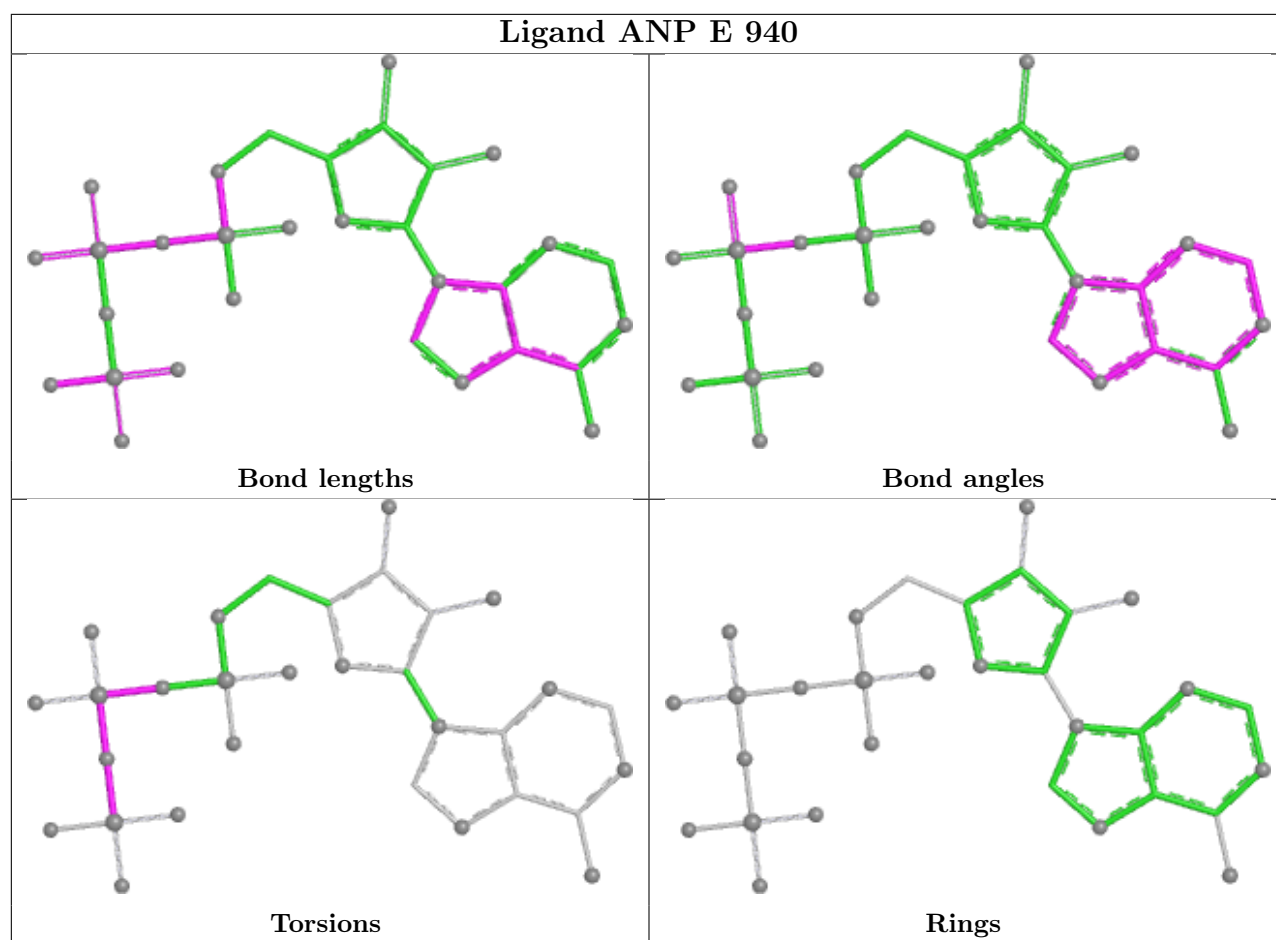
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	950	ANP	4	0
3	E	940	ANP	1	0
3	B	910	ANP	2	0
3	D	930	ANP	1	0

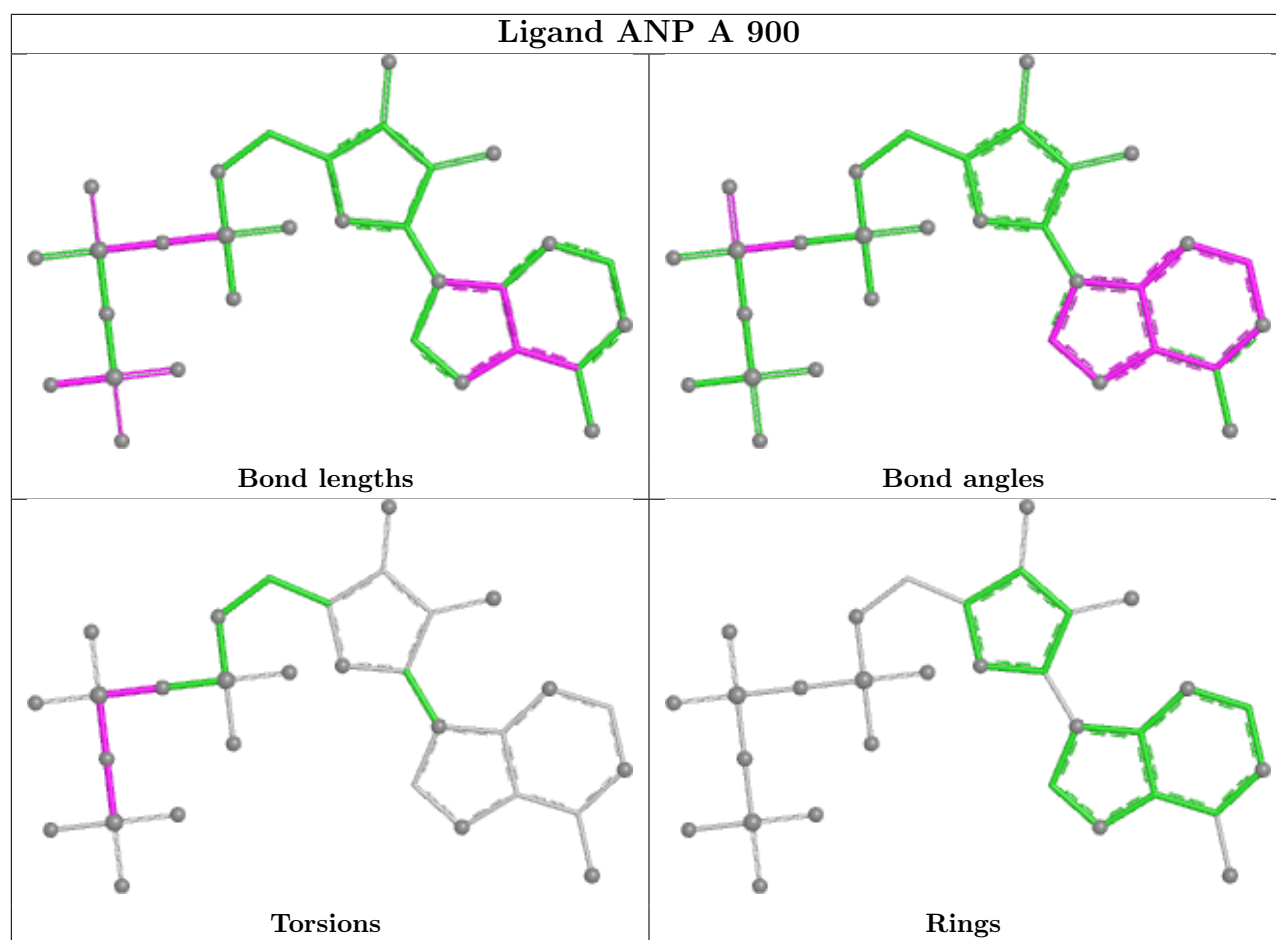
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

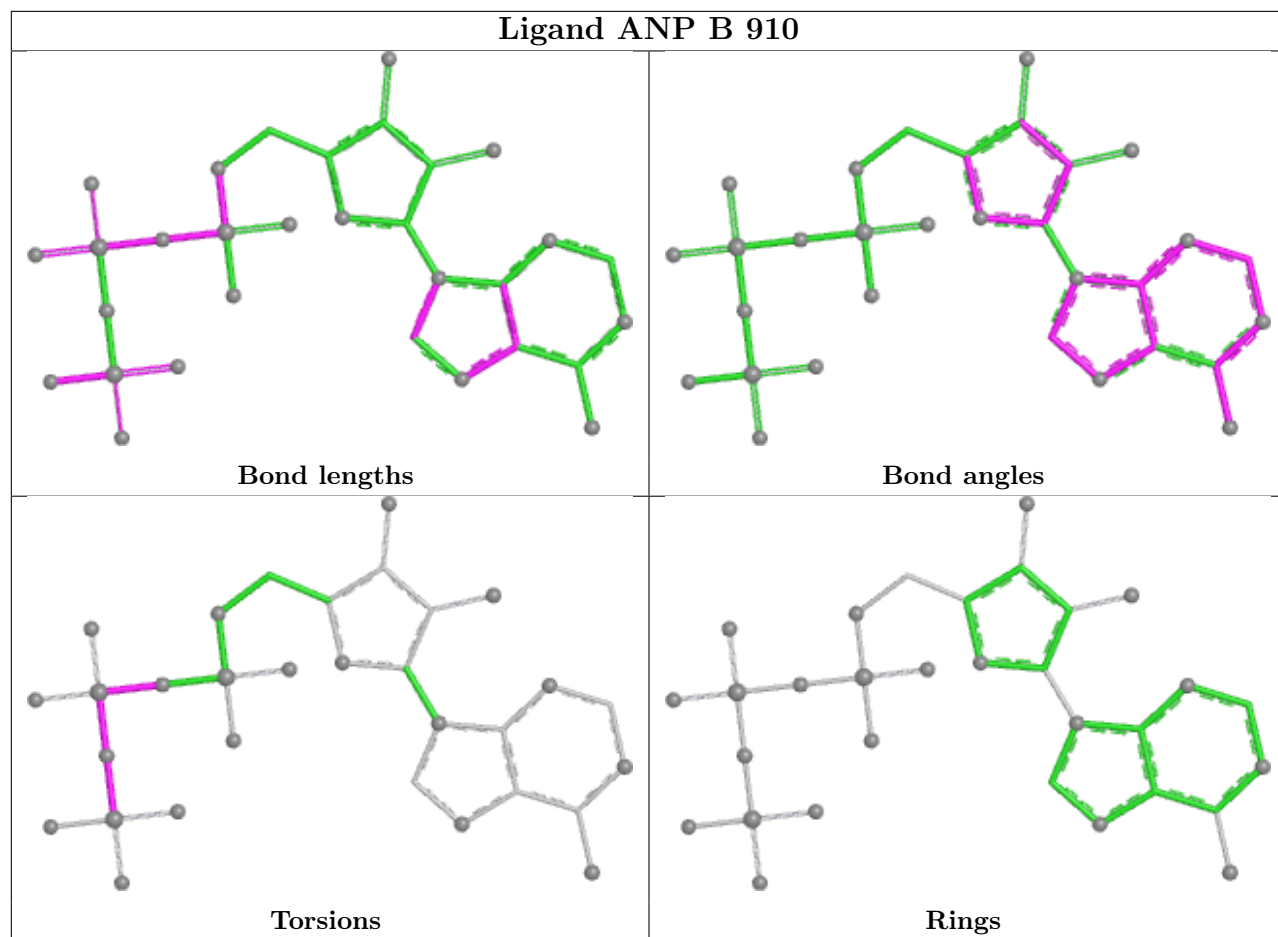
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

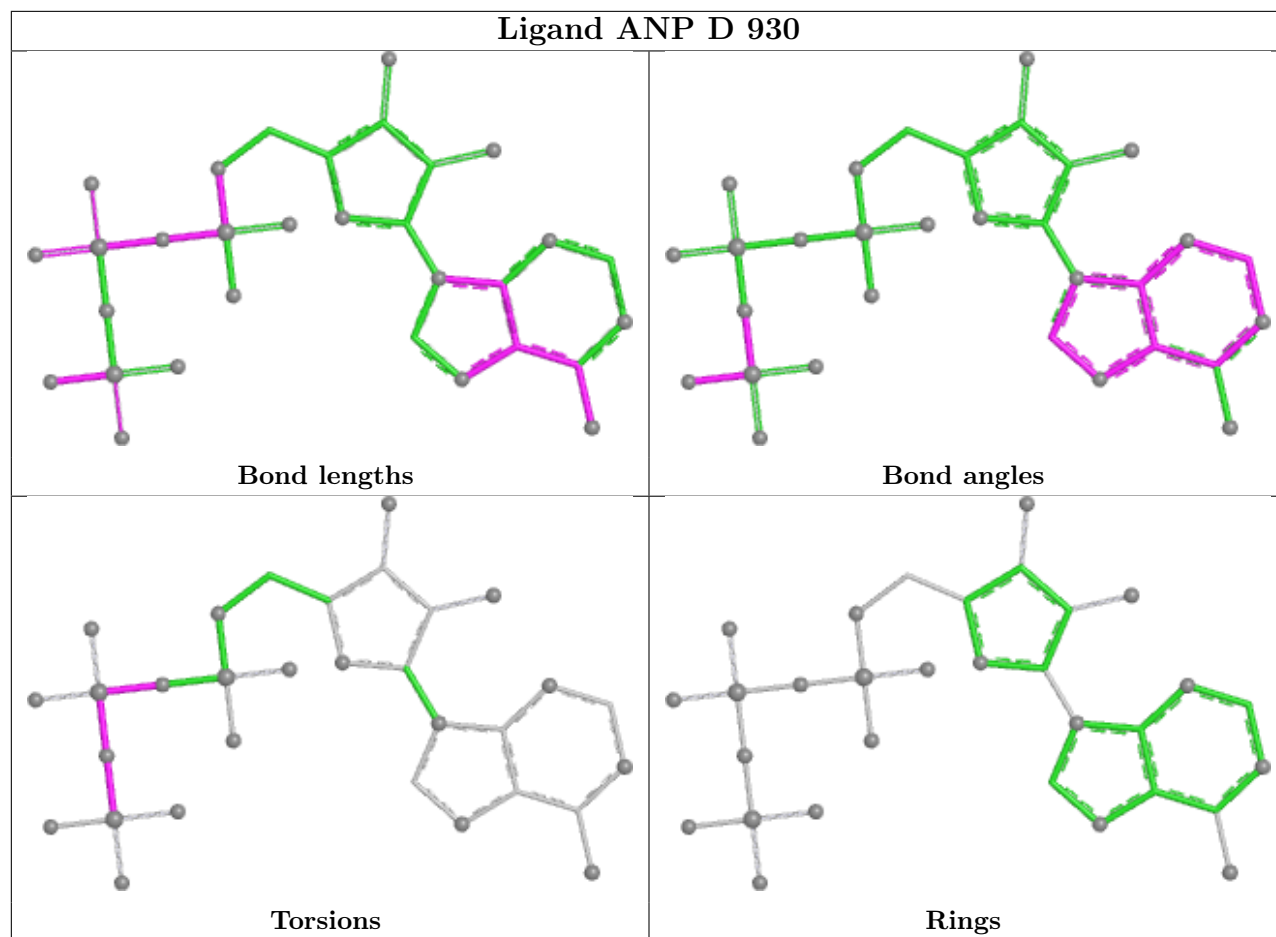












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	456/472 (96%)	-0.00	25 (5%)	30	32	4, 16, 48, 94	0
1	B	450/472 (95%)	-0.15	11 (2%)	59	62	4, 16, 40, 56	0
1	C	461/472 (97%)	-0.10	11 (2%)	59	62	7, 18, 39, 52	0
1	D	456/472 (96%)	-0.26	9 (1%)	65	66	4, 15, 37, 71	0
1	E	451/472 (95%)	0.08	16 (3%)	47	49	4, 18, 50, 72	0
1	F	449/472 (95%)	2.36	248 (55%)	0	0	18, 46, 72, 98	0
All	All	2723/2832 (96%)	0.31	320 (11%)	9	10	4, 19, 59, 98	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	212	VAL	7.9
1	F	211	ASN	7.2
1	F	217	ARG	7.1
1	F	162	GLU	6.9
1	F	159	GLY	6.7
1	F	62	LEU	6.6
1	F	207	ASP	6.5
1	F	174	ILE	6.3
1	F	358	PHE	6.2
1	F	156	VAL	6.1
1	F	222	ILE	6.1
1	F	183	ALA	5.9
1	F	127	ILE	5.8
1	F	208	PRO	5.8
1	D	461	GLU	5.7
1	F	213	THR	5.6
1	F	205	PHE	5.6
1	F	131	THR	5.4
1	F	160	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	63	ILE	5.3
1	F	180	TRP	5.2
1	E	167	PHE	5.2
1	F	334	PHE	5.2
1	F	60	ILE	5.1
1	F	320	ASP	5.1
1	F	163	ASN	5.0
1	B	164	THR	5.0
1	F	187	ILE	5.0
1	F	333	ASP	5.0
1	F	214	TYR	5.0
1	F	47	THR	5.0
1	F	132	SER	4.9
1	F	136	SER	4.9
1	F	133	PRO	4.9
1	F	52	ILE	4.9
1	F	140	TYR	4.9
1	F	216	PRO	4.8
1	F	154	ILE	4.8
1	F	7	PHE	4.8
1	F	455	LEU	4.8
1	F	39	LEU	4.7
1	F	203	PHE	4.7
1	D	464	ALA	4.7
1	F	197	ILE	4.7
1	A	464	ALA	4.7
1	F	215	TYR	4.6
1	F	56	ILE	4.6
1	F	139	ILE	4.6
1	F	109	GLY	4.6
1	F	218	LEU	4.6
1	F	85	GLU	4.5
1	F	399	ARG	4.5
1	F	53	LEU	4.4
1	F	148	ILE	4.4
1	F	172	VAL	4.4
1	F	170	THR	4.4
1	F	200	TYR	4.4
1	C	164	THR	4.3
1	F	196	ILE	4.3
1	F	130	GLU	4.3
1	F	158	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	169	GLY	4.3
1	F	75	VAL	4.3
1	F	164	THR	4.3
1	F	401	GLY	4.3
1	F	69	ILE	4.3
1	F	57	LYS	4.2
1	F	79	ILE	4.2
1	F	142	PHE	4.2
1	F	138	ARG	4.2
1	F	153	PRO	4.2
1	F	321	LEU	4.2
1	F	26	PRO	4.2
1	F	185	SER	4.1
1	F	451	LEU	4.1
1	F	141	THR	4.1
1	F	191	ILE	4.1
1	F	223	PRO	4.1
1	F	40	ILE	4.1
1	F	206	LYS	4.1
1	F	405	ASP	4.1
1	F	55	ASN	4.0
1	F	58	ILE	4.0
1	F	161	VAL	4.0
1	F	181	PRO	4.0
1	F	458	LYS	4.0
1	F	188	TYR	4.0
1	F	54	PRO	4.0
1	F	285	VAL	3.9
1	A	467	LYS	3.9
1	F	125	LYS	3.9
1	F	459	ARG	3.9
1	F	33	TYR	3.9
1	F	400	TYR	3.9
1	B	166	GLY	3.9
1	F	155	ILE	3.9
1	F	402	ILE	3.9
1	F	68	GLN	3.9
1	F	72	VAL	3.9
1	A	460	LYS	3.9
1	F	178	GLY	3.8
1	F	278	GLY	3.8
1	F	325	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	456	SER	3.8
1	F	157	GLU	3.7
1	C	407	TYR	3.7
1	F	194	THR	3.7
1	E	405	ASP	3.7
1	F	49	VAL	3.7
1	F	129	ILE	3.6
1	F	461	GLU	3.6
1	F	198	THR	3.6
1	F	29	ALA	3.6
1	F	201	ALA	3.6
1	F	204	ILE	3.6
1	F	454	TYR	3.5
1	B	167	PHE	3.5
1	F	219	THR	3.5
1	C	403	GLU	3.5
1	F	177	PRO	3.5
1	F	9	SER	3.5
1	F	408	GLN	3.5
1	F	168	HIS	3.5
1	F	324	LEU	3.5
1	F	28	PRO	3.4
1	F	128	GLU	3.4
1	F	317	ILE	3.4
1	F	61	ASP	3.4
1	F	45	ASP	3.4
1	F	282	ASN	3.3
1	F	81	ILE	3.3
1	F	462	GLN	3.3
1	F	110	LEU	3.3
1	F	289	THR	3.3
1	F	123	GLN	3.2
1	A	458	LYS	3.2
1	B	457	GLU	3.2
1	F	70	TYR	3.2
1	F	246	ASN	3.2
1	B	165	ARG	3.2
1	C	406	GLN	3.2
1	F	357	ALA	3.1
1	F	112	VAL	3.1
1	F	134	VAL	3.1
1	E	164	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	315	SER	3.1
1	F	404	SER	3.1
1	F	64	ASP	3.1
1	F	124	ASP	3.1
1	F	396	ASP	3.1
1	F	74	VAL	3.1
1	F	78	GLY	3.1
1	F	209	GLU	3.0
1	A	465	LYS	3.0
1	B	458	LYS	3.0
1	F	398	LYS	3.0
1	C	168	HIS	3.0
1	F	220	ASN	3.0
1	F	66	ALA	3.0
1	A	463	GLU	3.0
1	F	104	THR	3.0
1	F	184	LYS	3.0
1	B	135	ASN	3.0
1	A	395	LEU	3.0
1	F	176	ILE	3.0
1	E	4	LYS	3.0
1	F	453	GLN	3.0
1	F	190	TYR	3.0
1	F	80	GLY	3.0
1	D	462	GLN	2.9
1	F	30	ARG	2.9
1	B	252	TYR	2.9
1	F	48	ASP	2.9
1	F	76	ASP	2.9
1	C	167	PHE	2.9
1	A	462	GLN	2.9
1	A	407	TYR	2.9
1	F	51	GLY	2.9
1	F	95	TYR	2.9
1	C	165	ARG	2.8
1	F	252	TYR	2.8
1	F	362	ILE	2.8
1	F	175	SER	2.8
1	F	32	LEU	2.8
1	E	7	PHE	2.8
1	E	459	ARG	2.8
1	A	312	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	361	SER	2.8
1	F	89	ALA	2.8
1	E	168	HIS	2.8
1	F	369	ILE	2.8
1	A	406	GLN	2.8
1	F	426	GLY	2.8
1	F	35	THR	2.7
1	F	146	ILE	2.7
1	F	335	ALA	2.7
1	F	364	VAL	2.7
1	F	84	GLN	2.7
1	F	199	PRO	2.7
1	F	122	HIS	2.7
1	E	312	ASP	2.7
1	F	83	PRO	2.7
1	F	126	PRO	2.7
1	F	366	GLU	2.7
1	F	25	PHE	2.7
1	F	425	ALA	2.6
1	F	327	LYS	2.6
1	F	65	ASP	2.6
1	F	365	GLY	2.6
1	F	192	LYS	2.6
1	F	193	ARG	2.6
1	A	401	GLY	2.6
1	B	456	SER	2.6
1	D	403	GLU	2.6
1	F	67	ARG	2.6
1	F	254	ILE	2.6
1	F	4	LYS	2.6
1	F	255	LYS	2.6
1	F	312	ASP	2.6
1	F	316	VAL	2.6
1	F	407	TYR	2.6
1	F	44	LEU	2.5
1	F	173	ALA	2.5
1	F	77	ASN	2.5
1	F	91	GLY	2.5
1	F	294	THR	2.5
1	F	229	VAL	2.5
1	C	137	LYS	2.5
1	C	166	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	330	PHE	2.5
1	C	135	ASN	2.5
1	F	8	THR	2.4
1	F	434	GLU	2.4
1	B	137	LYS	2.4
1	F	186	ARG	2.4
1	F	359	GLY	2.4
1	F	463	GLU	2.4
1	F	257	PHE	2.4
1	F	296	LEU	2.4
1	F	31	ALA	2.4
1	F	310	SER	2.4
1	F	221	LYS	2.4
1	F	356	VAL	2.4
1	A	162	GLU	2.4
1	F	144	LEU	2.4
1	B	168	HIS	2.4
1	F	87	PRO	2.3
1	D	166	GLY	2.3
1	E	311	ALA	2.3
1	E	251	ASP	2.3
1	E	252	TYR	2.3
1	F	106	GLY	2.3
1	F	111	GLY	2.3
1	F	115	ALA	2.3
1	F	59	THR	2.3
1	D	459	ARG	2.3
1	F	90	PHE	2.3
1	F	256	GLU	2.3
1	F	101	ASN	2.3
1	F	182	LYS	2.3
1	E	313	SER	2.3
1	F	290	GLU	2.3
1	F	94	LEU	2.3
1	F	224	LYS	2.3
1	A	135	ASN	2.3
1	F	149	ASN	2.3
1	F	360	GLY	2.3
1	A	459	ARG	2.3
1	F	37	ARG	2.2
1	A	366	GLU	2.2
1	F	6	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	137	LYS	2.2
1	F	460	LYS	2.2
1	D	402	ILE	2.2
1	F	281	PRO	2.2
1	F	291	GLU	2.2
1	D	460	LYS	2.2
1	F	119	SER	2.2
1	F	447	VAL	2.2
1	A	402	ILE	2.2
1	F	395	LEU	2.2
1	F	5	GLU	2.2
1	A	163	ASN	2.1
1	F	73	ASN	2.1
1	F	50	HIS	2.1
1	F	311	ALA	2.1
1	F	276	LEU	2.1
1	F	322	ILE	2.1
1	F	393	GLU	2.1
1	A	447	VAL	2.1
1	F	397	TRP	2.1
1	F	313	SER	2.1
1	F	88	ASN	2.1
1	F	329	ILE	2.1
1	A	453	GLN	2.1
1	A	167	PHE	2.1
1	F	171	SER	2.1
1	F	253	THR	2.1
1	D	311	ALA	2.1
1	F	23	ALA	2.1
1	F	71	LYS	2.1
1	F	302	LYS	2.1
1	A	461	GLU	2.1
1	F	298	GLU	2.1
1	F	248	LEU	2.1
1	F	226	PRO	2.1
1	E	162	GLU	2.0
1	F	189	GLU	2.0
1	F	261	GLU	2.0
1	F	22	LEU	2.0
1	E	402	ILE	2.0
1	E	249	LYS	2.0
1	A	404	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	464	ALA	2.0
1	E	453	GLN	2.0
1	F	147	ASP	2.0
1	A	399	ARG	2.0
1	F	18	ARG	2.0
1	F	332	PRO	2.0
1	F	280	LYS	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.

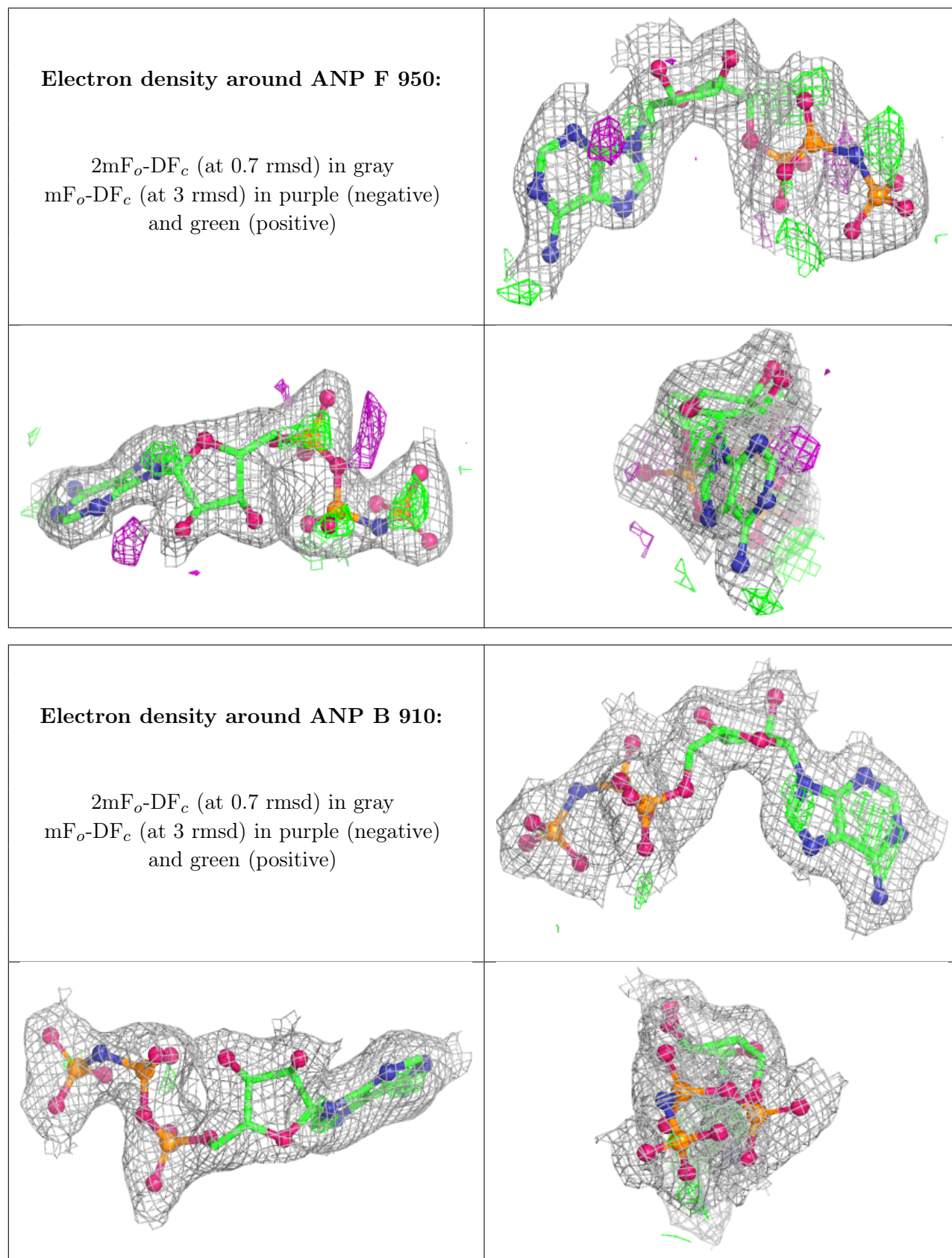
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	F	501	1/1	0.73	0.16	80,80,80,80	0
4	NA	D	901	1/1	0.82	0.21	78,78,78,78	0
3	ANP	F	950	31/31	0.89	0.17	59,76,78,78	0
2	MG	E	501	1/1	0.91	0.10	51,51,51,51	0
3	ANP	B	910	31/31	0.97	0.09	38,43,46,47	0
3	ANP	C	920	31/31	0.97	0.09	42,48,52,52	0
3	ANP	E	940	31/31	0.97	0.10	43,47,49,49	0
2	MG	B	501	1/1	0.97	0.11	42,42,42,42	0
2	MG	C	501	1/1	0.97	0.05	49,49,49,49	0
2	MG	D	501	1/1	0.98	0.06	45,45,45,45	0
3	ANP	A	900	31/31	0.98	0.09	40,45,47,47	0
3	ANP	D	930	31/31	0.98	0.09	41,45,48,48	0
2	MG	A	501	1/1	0.99	0.08	43,43,43,43	0

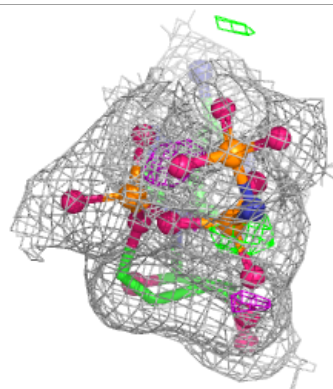
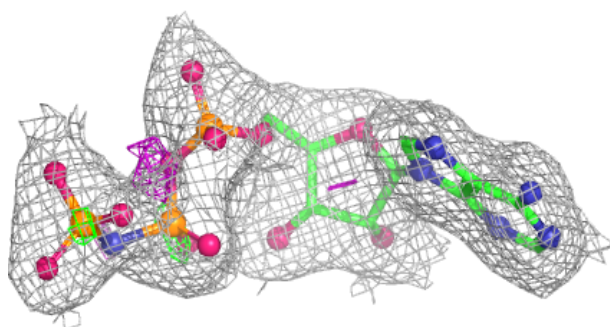
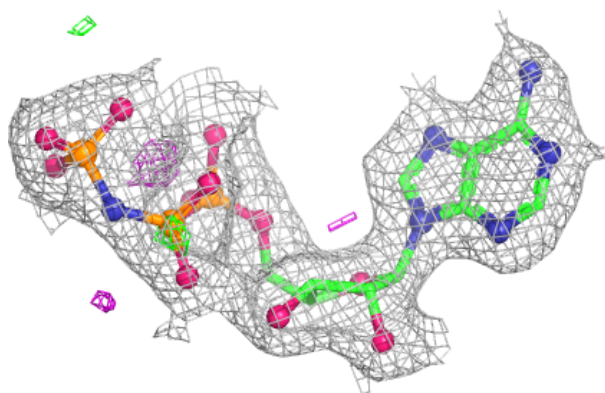
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

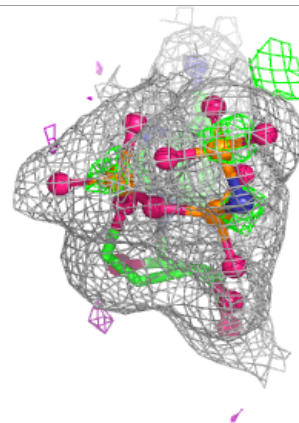
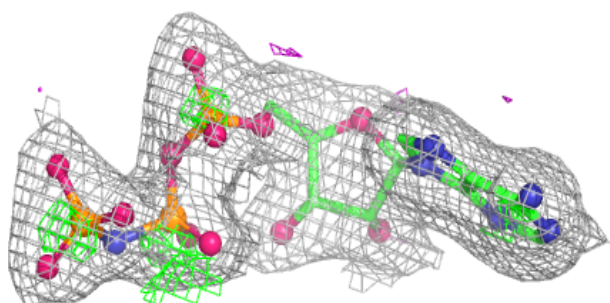
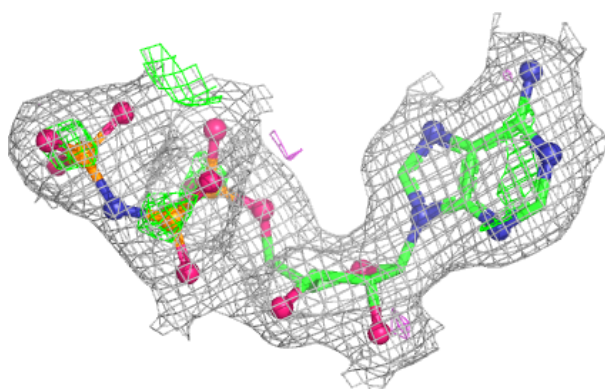


Electron density around ANP C 920:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

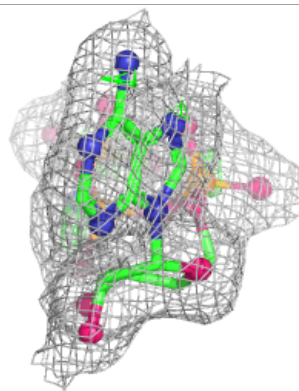
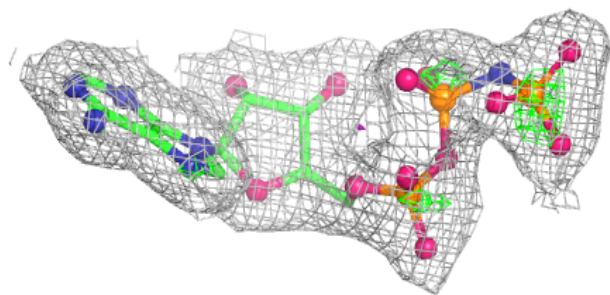
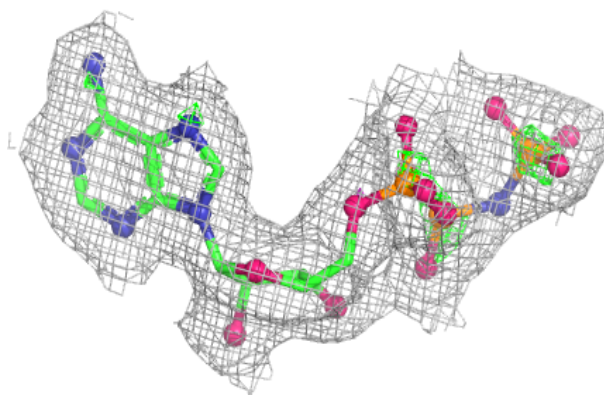
**Electron density around ANP E 940:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

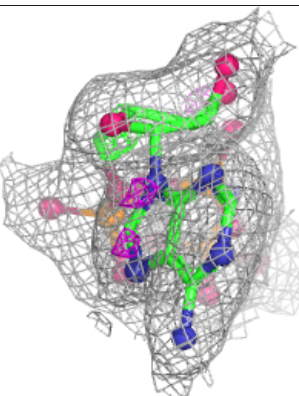
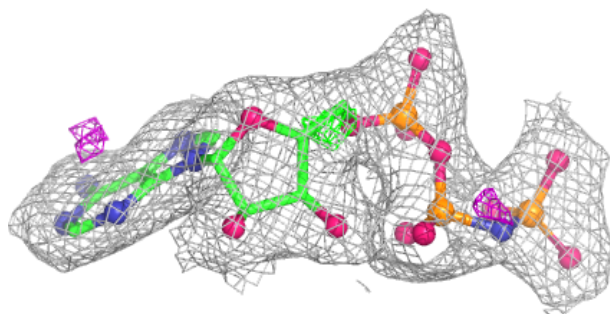
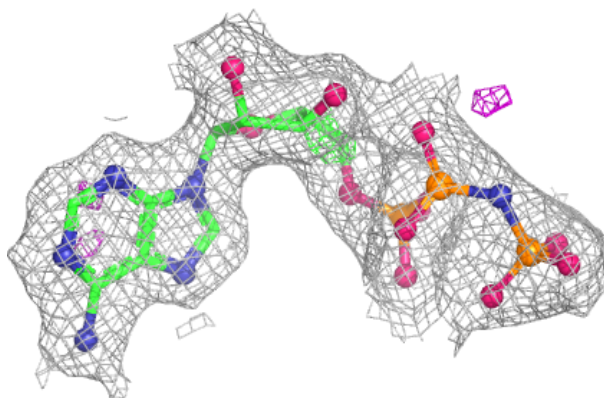


Electron density around ANP A 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ANP D 930:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.