



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:35 PM UTC

PDB ID : 4GFH / pdb_00004gfh
Title : Topoisomerase II-DNA-AMPPNP complex
Authors : Schmidt, B.H.; Osheroﬀ, N.; Berger, J.M.
Deposited on : 2012-08-03
Resolution : 4.41 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

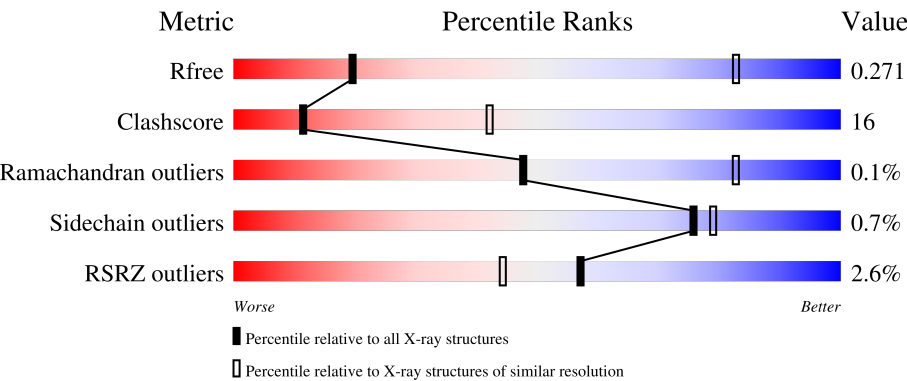
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.41 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	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	1178	2% 63% 29% • 6%
1	F	1178	2% 63% 29% • 7%
2	B	11	45% 55%
2	G	11	55% 45%
3	C	15	7% 60% 40%

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Mol	Chain	Length	Quality of chain
3	H	15	
4	D	11	
4	I	11	
5	E	15	
5	J	15	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PTR	F	782[A]	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA topoisomerase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1102	Total	C	N	O	P	S	0	1	0
			9042	5804	1515	1687	1	35			
1	F	1098	Total	C	N	O	P	S	0	1	0
			9012	5788	1510	1678	1	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	11	0
			219	105	36	67	11			
2	G	11	Total	C	N	O	P	0	11	0
			219	105	36	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	P	0	15	0
			310	147	63	86	14			
3	H	15	Total	C	N	O	P	0	15	0
			310	147	63	86	14			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*GP*AP*TP*GP*AP*CP*GP*AP*TP*(TSP))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	S	0	11	0
			230	109	44	65	11	1			
4	I	11	Total	C	N	O	P	S	0	11	0
			230	109	44	65	11	1			

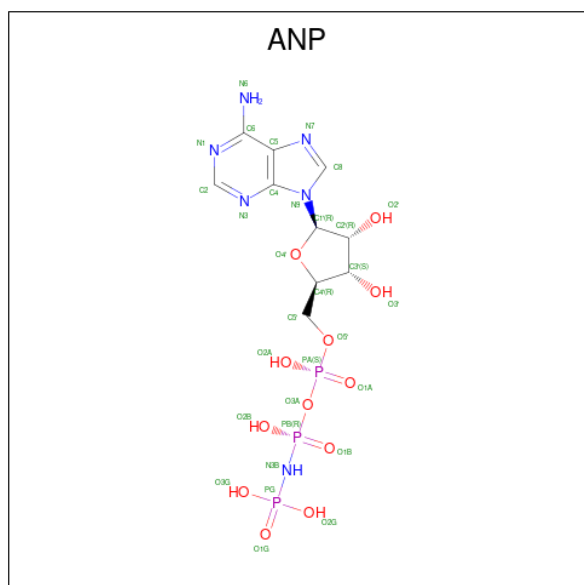
- Molecule 5 is a DNA chain called DNA (5'-D(*CP*GP*CP*GP*AP*AP*TP*CP*GP*TP*CP*AP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total	C	N	O	P	0	15	0
			300	144	54	88	14			
5	J	15	Total	C	N	O	P	0	15	0
			300	144	54	88	14			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

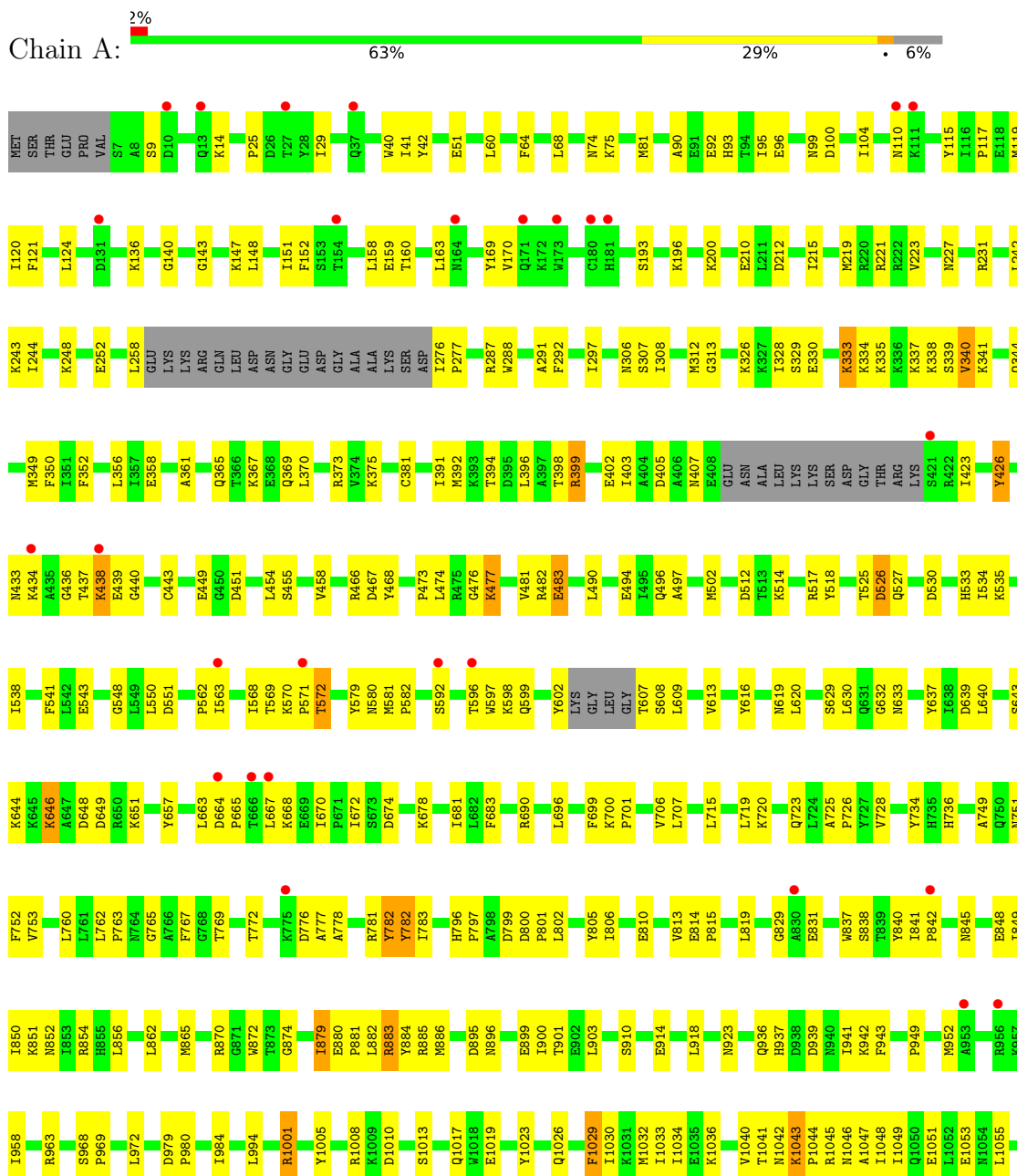
- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

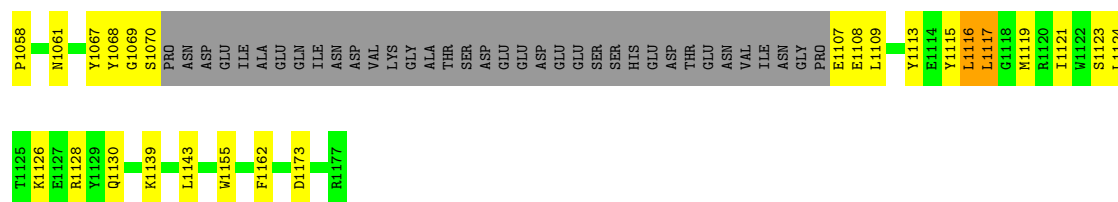


3 Residue-property plots

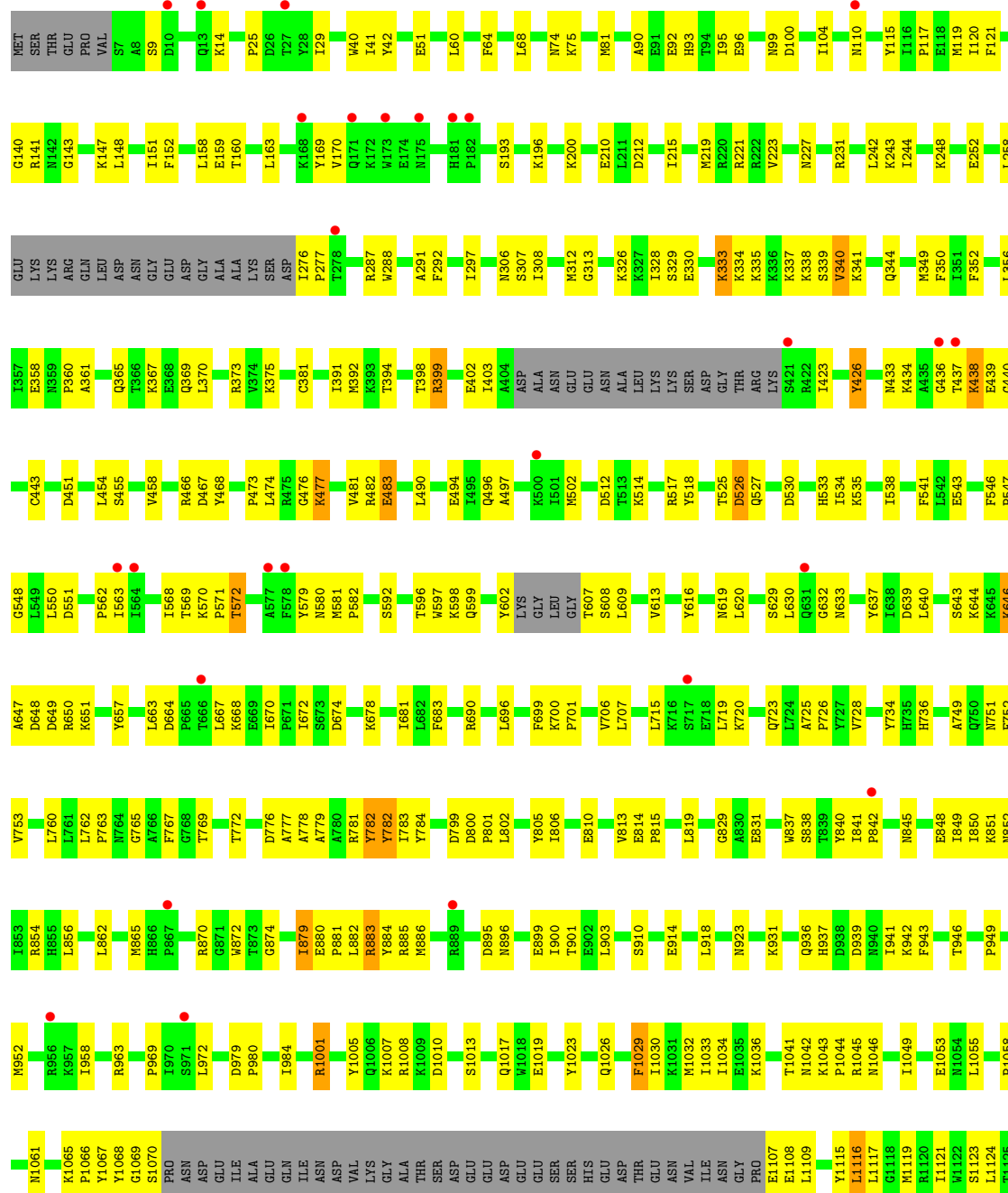
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA topoisomerase 2





• Molecule 1: DNA topoisomerase 2

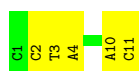




- Molecule 2: DNA (5'-D(P*CP*CP*TP*AP*CP*TP*GP*CP*TP*AP*C)-3')



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



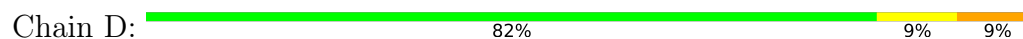
- Molecule 3: DNA (5'-D(*CP*GP*CP*GP*GP*TP*AP*GP*CP*AP*GP*TP*AP*GP*G)-3')



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



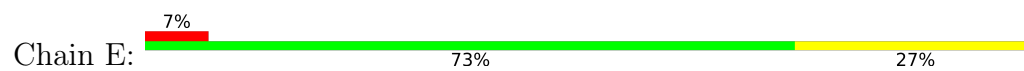
- Molecule 4: DNA (5'-D(P*GP*GP*AP*TP*GP*AP*CP*GP*AP*TP*(TSP))-3')



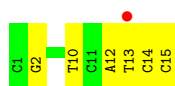
- Molecule 4: DNA (5'-D(P*GP*GP*AP*TP*GP*AP*CP*GP*AP*TP*(TSP))-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	169.13Å 169.88Å 169.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 4.41 46.99 – 4.41	Depositor EDS
% Data completeness (in resolution range)	91.2 (46.99-4.41) 90.9 (46.99-4.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 4.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.239 , 0.275 0.236 , 0.271	Depositor DCC
R_{free} test set	1458 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	185.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 875.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -k,-h,l 0.389 for l,-k,h 0.000 for l,h,k 0.000 for k,l,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20236	wwPDB-VP
Average B, all atoms (Å ²)	248.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, TSP, ANP, 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	0.28	0/9218	0.78	19/12428 (0.2%)
1	F	0.28	0/9188	0.78	19/12387 (0.2%)
2	B	0.25	0/243	0.55	0/371
2	G	0.24	0/243	0.57	0/371
3	C	0.31	0/349	0.52	0/539
3	H	0.21	0/349	0.55	0/539
4	D	0.24	0/236	0.70	2/363 (0.6%)
4	I	0.23	0/236	0.83	2/363 (0.6%)
5	E	0.19	0/335	0.54	0/514
5	J	0.19	0/335	0.53	0/514
All	All	0.27	0/20732	0.76	42/28389 (0.1%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	879	ILE	CB-CA-C	-11.30	100.45	111.30
1	F	879	ILE	CB-CA-C	-11.27	100.48	111.30
4	I	10[B]	DT	C4'-C3'-O3'	10.09	125.13	110.00
1	A	696	LEU	N-CA-C	9.09	120.96	111.14
1	F	696	LEU	N-CA-C	9.08	120.95	111.14
1	A	438	LYS	N-CA-C	-8.13	103.11	112.87
1	F	438	LYS	N-CA-C	-8.12	103.12	112.87
1	A	1029	PHE	N-CA-C	6.97	118.67	111.14
1	F	1029	PHE	N-CA-C	6.96	118.66	111.14
1	A	340	VAL	N-CA-C	6.96	118.07	110.21
1	F	340	VAL	N-CA-C	6.93	118.05	110.21
1	A	1117	LEU	N-CA-C	-6.74	105.21	113.50
1	F	1117	LEU	N-CA-C	-6.74	105.21	113.50
1	A	494	GLU	N-CA-C	6.69	118.36	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	494	GLU	N-CA-C	6.66	118.34	111.14
4	D	10[B]	DT	C2'-C3'-O3'	-6.43	101.85	111.50
1	A	569	THR	N-CA-C	6.33	121.10	112.68
1	F	569	THR	N-CA-C	6.30	121.06	112.68
4	I	10[B]	DT	C2'-C3'-O3'	-6.24	102.14	111.50
1	A	939	ASP	N-CA-C	-5.51	107.13	112.97
1	F	939	ASP	N-CA-C	-5.47	107.17	112.97
1	F	483	GLU	CB-CA-C	-5.45	104.22	111.63
1	A	483	GLU	CB-CA-C	-5.41	104.27	111.63
1	F	426	TYR	CA-C-N	5.38	124.56	118.97
1	F	426	TYR	C-N-CA	5.38	124.56	118.97
1	A	426	TYR	CA-C-N	5.38	124.56	118.97
1	A	426	TYR	C-N-CA	5.38	124.56	118.97
1	F	646	LYS	N-CA-C	5.37	119.35	112.26
1	A	646	LYS	N-CA-C	5.37	119.34	112.26
1	F	477	LYS	N-CA-C	-5.34	102.14	110.10
1	A	477	LYS	N-CA-C	-5.32	102.18	110.10
4	D	10[B]	DT	C4'-C3'-O3'	5.31	117.97	110.00
1	A	1116	LEU	N-CA-C	5.27	121.11	114.31
1	A	772	THR	CB-CA-C	-5.25	102.25	110.85
1	F	1116	LEU	N-CA-C	5.24	121.07	114.31
1	A	1116	LEU	CB-CA-C	-5.24	100.22	109.02
1	F	772	THR	CB-CA-C	-5.24	102.26	110.85
1	F	1116	LEU	CB-CA-C	-5.23	100.23	109.02
1	F	1043	LYS	N-CA-C	5.18	121.25	109.81
1	A	1043	LYS	N-CA-C	5.16	121.22	109.81
1	F	572	THR	N-CA-C	-5.11	100.98	108.79
1	A	572	THR	N-CA-C	-5.07	101.04	108.79

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	9042	0	9077	324	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	9012	0	9056	318	0
2	B	219	0	114	6	0
2	G	219	0	118	6	0
3	C	310	0	146	5	0
3	H	310	0	147	7	0
4	D	230	0	108	1	0
4	I	230	0	108	6	0
5	E	300	0	154	3	0
5	J	300	0	153	7	0
6	A	1	0	0	0	0
6	F	1	0	0	0	0
7	A	31	0	13	2	0
7	F	31	0	13	2	0
All	All	20236	0	19207	632	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 16.

All (632) 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:F:29:ILE:HD13	1:F:152:PHE:CE2	1.73	1.24
1:A:29:ILE:HD13	1:A:152:PHE:CE2	1.73	1.23
1:F:29:ILE:CD1	1:F:152:PHE:CZ	2.38	1.06
1:A:29:ILE:CD1	1:A:152:PHE:CZ	2.38	1.05
1:A:29:ILE:HD13	1:A:152:PHE:CZ	1.93	1.02
1:F:29:ILE:HD13	1:F:152:PHE:CZ	1.93	1.01
1:A:74:ASN:HB3	1:A:81:MET:HE1	1.45	0.98
1:F:74:ASN:HB3	1:F:81:MET:HE1	1.44	0.98
1:F:778:ALA:HB1	1:F:782[A]:PTR:HD1	1.47	0.95
1:A:276:ILE:HG12	1:A:394:THR:HG22	1.50	0.94
1:F:437:THR:HG22	1:F:438:LYS:H	1.32	0.94
1:A:437:THR:HG22	1:A:438:LYS:H	1.32	0.93
1:F:29:ILE:HD11	1:F:152:PHE:CZ	2.05	0.92
1:F:276:ILE:HG12	1:F:394:THR:HG22	1.50	0.91
1:A:29:ILE:HD11	1:A:152:PHE:CZ	2.05	0.90
1:A:333:LYS:HG3	1:A:339:SER:HB3	1.54	0.89
1:F:333:LYS:HG3	1:F:339:SER:HB3	1.54	0.88
1:F:879:ILE:HD11	1:F:885:ARG:HG3	1.55	0.88
1:A:879:ILE:HD11	1:A:885:ARG:HG3	1.55	0.88
1:A:291:ALA:HB3	1:A:352:PHE:HB2	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:ALA:HB3	1:F:352:PHE:HB2	1.58	0.84
1:A:1032:MET:HE1	1:A:1055:LEU:HD13	1.60	0.83
1:F:1032:MET:HE1	1:F:1055:LEU:HD13	1.60	0.83
1:A:778:ALA:HB1	1:A:782[A]:PTR:HD1	1.64	0.79
1:F:437:THR:CG2	1:F:438:LYS:H	1.96	0.79
1:F:454:LEU:HD22	1:F:473:PRO:HG3	1.66	0.78
1:A:454:LEU:HD22	1:A:473:PRO:HG3	1.66	0.78
1:A:437:THR:CG2	1:A:438:LYS:H	1.96	0.77
1:A:633:ASN:O	1:A:637:TYR:HD1	1.68	0.76
1:F:570:LYS:HB2	1:F:596:THR:OG1	1.87	0.75
1:A:570:LYS:HB2	1:A:596:THR:OG1	1.85	0.75
1:F:633:ASN:O	1:F:637:TYR:HD1	1.68	0.75
1:A:276:ILE:CG1	1:A:394:THR:HG22	2.17	0.74
1:F:437:THR:HG22	1:F:438:LYS:N	2.02	0.74
1:A:436:GLY:HA2	1:A:517:ARG:HA	1.70	0.74
1:A:437:THR:HG22	1:A:438:LYS:N	2.02	0.73
1:F:436:GLY:HA2	1:F:517:ARG:HA	1.70	0.73
1:F:276:ILE:CG1	1:F:394:THR:HG22	2.17	0.73
1:A:725:ALA:HB3	1:A:726:PRO:HD3	1.70	0.73
1:A:850:ILE:HG22	1:A:854:ARG:NH1	2.04	0.72
1:F:292:PHE:HE1	1:F:349:MET:HG2	1.55	0.72
1:F:725:ALA:HB3	1:F:726:PRO:HD3	1.70	0.71
1:A:399:ARG:HG3	1:A:399:ARG:HH11	1.56	0.71
1:F:850:ILE:HG22	1:F:854:ARG:NH1	2.04	0.71
1:F:481:VAL:HG11	1:F:541:PHE:HD1	1.56	0.71
1:A:292:PHE:HE1	1:A:349:MET:HG2	1.55	0.70
1:A:481:VAL:HG11	1:A:541:PHE:HD1	1.56	0.70
1:A:856:LEU:HG	1:A:862:LEU:HD21	1.74	0.69
1:A:936:GLN:O	1:A:942:LYS:HB2	1.93	0.69
1:F:399:ARG:HG3	1:F:399:ARG:HH11	1.56	0.69
1:F:936:GLN:O	1:F:942:LYS:HB2	1.93	0.69
1:F:856:LEU:HG	1:F:862:LEU:HD21	1.74	0.68
1:A:936:GLN:O	1:A:942:LYS:CB	2.42	0.68
1:F:936:GLN:O	1:F:942:LYS:CB	2.42	0.67
1:A:831:GLU:HG3	1:A:840:TYR:HD1	1.60	0.67
1:F:831:GLU:HG3	1:F:840:TYR:HD1	1.60	0.67
1:F:620:LEU:HD23	1:F:620:LEU:H	1.60	0.66
1:F:399:ARG:HH11	1:F:399:ARG:CG	2.09	0.66
1:A:399:ARG:HH11	1:A:399:ARG:CG	2.09	0.65
1:F:668:LYS:O	1:F:668:LYS:HG3	1.96	0.65
1:A:571:PRO:HD3	1:A:596:THR:OG1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:LYS:O	1:A:668:LYS:HG3	1.96	0.65
1:A:726:PRO:HG2	1:F:726:PRO:HG2	1.78	0.65
1:F:571:PRO:HD3	1:F:596:THR:OG1	1.97	0.65
1:A:752:PHE:O	1:A:753:VAL:C	2.40	0.65
4:I:1[B]:DG:N2	5:J:15[B]:DC:O2	2.29	0.65
1:F:1058:PRO:HB3	1:F:1068:TYR:CD1	2.32	0.65
1:A:1058:PRO:HB3	1:A:1068:TYR:CD1	2.32	0.64
1:A:512:ASP:HB3	1:A:514:LYS:HG2	1.79	0.64
1:F:512:ASP:HB3	1:F:514:LYS:HG2	1.79	0.64
1:A:620:LEU:HD23	1:A:620:LEU:H	1.61	0.64
1:A:525:THR:OG1	1:A:535:LYS:HE3	1.98	0.64
1:A:715:LEU:HD11	1:A:719:LEU:HD22	1.80	0.64
1:A:767:PHE:CE1	1:A:783:ILE:HB	2.33	0.64
1:F:215:ILE:O	1:F:219:MET:HG3	1.98	0.64
1:F:525:THR:OG1	1:F:535:LYS:HE3	1.98	0.64
1:F:767:PHE:CE1	1:F:783:ILE:HB	2.33	0.63
1:F:881:PRO:O	1:F:882:LEU:HB2	1.98	0.63
1:A:881:PRO:O	1:A:882:LEU:HB2	1.98	0.63
1:F:715:LEU:HD11	1:F:719:LEU:HD22	1.80	0.63
1:F:903:LEU:HG	1:F:941:ILE:HD13	1.81	0.63
1:A:215:ILE:O	1:A:219:MET:HG3	1.98	0.62
1:F:344:GLN:OE1	1:F:403:ILE:HG21	1.99	0.62
1:F:782[A]:PTR:HE2	1:F:782[A]:PTR:O1P	1.99	0.62
1:F:1058:PRO:HB3	1:F:1068:TYR:CE1	2.35	0.62
1:A:344:GLN:OE1	1:A:403:ILE:HG21	1.99	0.62
1:A:903:LEU:HG	1:A:941:ILE:HD13	1.81	0.62
1:A:1058:PRO:HB3	1:A:1068:TYR:CE1	2.35	0.62
1:F:752:PHE:O	1:F:753:VAL:C	2.40	0.62
1:F:849:ILE:HA	1:F:865:MET:HE1	1.83	0.61
1:A:481:VAL:HG11	1:A:541:PHE:CD1	2.36	0.61
1:F:690:ARG:HD2	4:I:10[B]:DT:H5'	1.82	0.61
1:A:1029:PHE:O	1:A:1033:ILE:HG13	2.01	0.61
1:A:340:VAL:HG11	1:A:344:GLN:OE1	2.01	0.60
1:F:340:VAL:HG11	1:F:344:GLN:OE1	2.01	0.60
1:A:849:ILE:HA	1:A:865:MET:HE1	1.83	0.60
1:A:619:ASN:OD1	1:A:619:ASN:O	2.20	0.60
1:F:619:ASN:OD1	1:F:619:ASN:O	2.20	0.60
1:F:958:ILE:HD12	1:F:963:ARG:HD2	1.83	0.60
2:G:2[A]:DC:C6	2:G:3[A]:DT:H72	2.36	0.60
1:A:223:VAL:HG12	1:A:242:LEU:HD11	1.84	0.60
1:A:482:ARG:NH2	1:A:639:ASP:HA	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:SER:O	1:A:630:LEU:C	2.45	0.60
1:F:223:VAL:HG12	1:F:242:LEU:HD11	1.84	0.60
1:F:1029:PHE:O	1:F:1033:ILE:HG13	2.01	0.60
1:A:330:GLU:O	1:A:334:LYS:HB2	2.02	0.59
1:F:227:ASN:HD22	1:F:242:LEU:HB2	1.67	0.59
1:F:454:LEU:HD22	1:F:473:PRO:CG	2.31	0.59
1:A:958:ILE:HD12	1:A:963:ARG:HD2	1.83	0.59
1:F:482:ARG:NH2	1:F:639:ASP:HA	2.17	0.59
1:A:802:LEU:HD11	1:A:1008:ARG:HB2	1.84	0.59
1:F:481:VAL:HG11	1:F:541:PHE:CD1	2.36	0.59
1:F:571:PRO:HD3	1:F:596:THR:HG1	1.66	0.59
1:F:629:SER:O	1:F:630:LEU:C	2.45	0.59
1:F:1030:ILE:HG23	1:F:1124:LEU:HD23	1.85	0.59
1:A:227:ASN:HD22	1:A:242:LEU:HB2	1.67	0.58
1:F:276:ILE:HD12	1:F:277:PRO:HD2	1.86	0.58
1:A:454:LEU:HD22	1:A:473:PRO:CG	2.31	0.58
1:F:29:ILE:HD11	1:F:152:PHE:CE1	2.38	0.58
1:F:433:ASN:HB2	1:F:467:ASP:HA	1.85	0.58
1:F:330:GLU:O	1:F:334:LYS:HB2	2.03	0.58
1:F:592:SER:HB2	1:F:597:TRP:CZ2	2.39	0.58
1:F:802:LEU:HD11	1:F:1008:ARG:HB2	1.84	0.58
1:A:749:ALA:O	1:A:763:PRO:HG3	2.04	0.58
1:A:29:ILE:HD11	1:A:152:PHE:CE1	2.38	0.58
1:F:1123:SER:HA	1:F:1128:ARG:HB3	1.85	0.58
1:A:437:THR:O	1:A:440:GLY:N	2.37	0.57
1:A:592:SER:HB2	1:A:597:TRP:CZ2	2.39	0.57
1:F:749:ALA:O	1:F:763:PRO:HG3	2.04	0.57
1:F:776:ASP:N	1:F:776:ASP:OD1	2.35	0.57
1:F:1069:GLY:O	1:F:1070:SER:CB	2.53	0.57
1:A:140:GLY:HA2	7:A:1202:ANP:O2G	2.04	0.57
1:A:1030:ILE:HG23	1:A:1124:LEU:HD23	1.85	0.57
1:A:1123:SER:HA	1:A:1128:ARG:HB3	1.85	0.57
1:F:140:GLY:HA2	7:F:1202:ANP:O2G	2.04	0.57
1:F:720:LYS:HG2	1:F:723:GLN:CD	2.30	0.57
1:F:1067:TYR:CE1	1:F:1070:SER:N	2.73	0.57
1:F:328:ILE:HG12	1:F:392:MET:HE1	1.86	0.57
1:A:433:ASN:HB2	1:A:467:ASP:HA	1.85	0.57
1:F:437:THR:O	1:F:440:GLY:N	2.37	0.57
1:A:1067:TYR:CE1	1:A:1070:SER:N	2.73	0.57
1:A:1069:GLY:O	1:A:1070:SER:CB	2.53	0.57
1:A:328:ILE:HG12	1:A:392:MET:HE1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLN:OE1	1:A:403:ILE:HD13	2.05	0.56
1:A:720:LYS:HG2	1:A:723:GLN:CD	2.30	0.56
1:F:632:GLY:O	1:F:633:ASN:HB2	2.05	0.56
1:F:344:GLN:OE1	1:F:403:ILE:HD13	2.06	0.56
1:F:752:PHE:HD1	1:F:753:VAL:O	1.89	0.56
1:F:782[A]:PTR:O1P	1:F:782[A]:PTR:CE2	2.51	0.56
1:F:306:ASN:O	1:F:307:SER:HB2	2.05	0.56
1:F:437:THR:C	1:F:439:GLU:N	2.62	0.56
1:A:306:ASN:O	1:A:307:SER:HB2	2.05	0.56
1:A:276:ILE:HD12	1:A:277:PRO:HD2	1.86	0.56
1:A:437:THR:C	1:A:439:GLU:N	2.62	0.56
1:A:831:GLU:CG	1:A:840:TYR:HD1	2.18	0.56
1:A:979:ASP:HB2	1:A:980:PRO:HD2	1.88	0.56
1:A:657:TYR:HB2	1:A:681:ILE:CD1	2.36	0.56
1:F:455:SER:O	1:F:458:VAL:HG22	2.06	0.56
1:F:699:PHE:CZ	1:F:707:LEU:HD12	2.41	0.56
1:A:455:SER:O	1:A:458:VAL:HG22	2.06	0.56
1:A:466:ARG:NH1	1:F:937:HIS:H	2.04	0.55
1:F:437:THR:C	1:F:439:GLU:H	2.14	0.55
1:F:548:GLY:HA2	1:F:551:ASP:OD2	2.06	0.55
1:F:657:TYR:HB2	1:F:681:ILE:CD1	2.36	0.55
1:F:781:ARG:NH1	1:F:782[A]:PTR:O3P	2.39	0.55
1:A:1030:ILE:O	1:A:1034:ILE:HG13	2.07	0.55
3:C:14[A]:DG:H2''	3:C:15[A]:DG:OP2	2.06	0.55
1:F:434:LYS:HD3	1:F:439:GLU:CD	2.31	0.55
1:F:831:GLU:CG	1:F:840:TYR:HD1	2.18	0.55
1:A:752:PHE:HD1	1:A:753:VAL:O	1.89	0.55
1:A:632:GLY:O	1:A:633:ASN:HB2	2.05	0.55
1:A:434:LYS:HD3	1:A:439:GLU:CD	2.31	0.55
1:A:548:GLY:HA2	1:A:551:ASP:OD2	2.06	0.55
1:A:776:ASP:OD1	1:A:776:ASP:N	2.35	0.55
1:A:699:PHE:CZ	1:A:707:LEU:HD12	2.41	0.55
1:F:104:ILE:HB	1:F:160:THR:HG21	1.89	0.55
1:A:437:THR:C	1:A:439:GLU:H	2.14	0.54
1:F:979:ASP:HB2	1:F:980:PRO:HD2	1.88	0.54
1:F:1067:TYR:CZ	1:F:1069:GLY:HA3	2.42	0.54
1:A:690:ARG:HD2	4:D:10[B]:DT:H5'	1.90	0.54
1:F:563:ILE:HD12	1:F:580:ASN:HA	1.90	0.54
1:A:308:ILE:HD13	1:A:367:LYS:HD2	1.90	0.54
1:F:340:VAL:HG12	1:F:341:LYS:N	2.23	0.54
4:I:2[B]:DG:O6	5:J:14[B]:DC:N4	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:HB	1:A:160:THR:HG21	1.89	0.54
1:A:338:LYS:HD3	1:A:407:ASN:O	2.08	0.54
1:A:1119:MET:O	1:F:1121:ILE:HG13	2.08	0.54
1:F:1030:ILE:O	1:F:1034:ILE:HG13	2.07	0.54
1:A:563:ILE:O	1:A:602:TYR:HB2	2.08	0.53
1:A:563:ILE:HD12	1:A:580:ASN:HA	1.90	0.53
1:F:657:TYR:HB2	1:F:681:ILE:HD13	1.90	0.53
1:F:805:TYR:CE2	1:F:815:PRO:HG3	2.43	0.53
1:A:657:TYR:HB2	1:A:681:ILE:HD13	1.90	0.53
1:A:805:TYR:CE2	1:A:815:PRO:HG3	2.43	0.53
1:F:227:ASN:HB3	1:F:244:ILE:HD11	1.91	0.53
1:A:1067:TYR:CZ	1:A:1069:GLY:HA3	2.42	0.53
1:F:333:LYS:CA	1:F:339:SER:HB2	2.38	0.53
1:A:74:ASN:CB	1:A:81:MET:HE1	2.30	0.53
1:A:340:VAL:HG12	1:A:341:LYS:N	2.24	0.53
1:F:333:LYS:HG3	1:F:339:SER:CB	2.33	0.53
1:A:937:HIS:H	1:F:466:ARG:NH1	2.07	0.53
1:F:563:ILE:O	1:F:602:TYR:HB2	2.08	0.53
1:F:838:SER:HB3	5:J:10[B]:DT:H5'	1.90	0.53
1:F:805:TYR:HA	1:F:815:PRO:HA	1.91	0.53
1:A:227:ASN:HB3	1:A:244:ILE:HD11	1.91	0.52
1:A:423:ILE:HD11	1:A:517:ARG:HH22	1.74	0.52
1:A:581:MET:HB2	1:A:582:PRO:HD3	1.91	0.52
1:F:227:ASN:CG	1:F:244:ILE:HG13	2.35	0.52
1:F:734:TYR:CE2	1:F:736:HIS:HB2	2.43	0.52
1:F:568:ILE:HG22	1:F:572:THR:O	2.10	0.52
1:F:707:LEU:HD11	1:F:760:LEU:HD13	1.91	0.52
1:A:333:LYS:CA	1:A:339:SER:HB2	2.38	0.52
1:F:248:LYS:HE2	1:F:252:GLU:OE2	2.10	0.52
1:A:805:TYR:HA	1:A:815:PRO:HA	1.91	0.52
1:F:308:ILE:HD13	1:F:367:LYS:HD2	1.90	0.52
1:F:526:ASP:O	1:F:527:GLN:HB3	2.10	0.52
1:F:423:ILE:HD11	1:F:517:ARG:HH22	1.74	0.52
1:F:527:GLN:O	1:F:527:GLN:HG3	2.10	0.52
1:F:333:LYS:HA	1:F:339:SER:HB2	1.92	0.52
1:A:640:LEU:HA	1:A:646:LYS:HD2	1.92	0.52
1:A:707:LEU:HD11	1:A:760:LEU:HD13	1.91	0.52
1:A:734:TYR:CE2	1:A:736:HIS:HB2	2.43	0.51
1:A:1121:ILE:HG13	1:F:1119:MET:O	2.09	0.51
1:A:227:ASN:CG	1:A:244:ILE:HG13	2.35	0.51
1:F:581:MET:HB2	1:F:582:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HE2	1:A:252:GLU:OE2	2.10	0.51
1:F:648:ASP:HA	1:F:651:LYS:HD2	1.93	0.51
1:A:526:ASP:O	1:A:527:GLN:HB3	2.10	0.51
1:F:276:ILE:HD12	1:F:277:PRO:CD	2.41	0.51
1:A:288:TRP:CG	1:A:381:CYS:HB2	2.46	0.51
1:A:663:LEU:HD21	1:A:670:ILE:HG23	1.92	0.51
1:A:936:GLN:O	1:A:942:LYS:HB3	2.10	0.51
1:F:751:ASN:CG	1:F:763:PRO:HG2	2.36	0.51
1:A:437:THR:O	1:A:439:GLU:N	2.44	0.51
1:A:436:GLY:HA3	1:A:517:ARG:HD2	1.93	0.51
1:A:568:ILE:HG22	1:A:572:THR:O	2.10	0.51
1:A:148:LEU:O	1:A:152:PHE:HD2	1.94	0.51
1:A:333:LYS:HG3	1:A:339:SER:CB	2.33	0.51
1:A:333:LYS:HA	1:A:339:SER:HB2	1.92	0.51
1:A:527:GLN:O	1:A:527:GLN:HG3	2.10	0.51
1:A:648:ASP:HA	1:A:651:LYS:HD2	1.93	0.51
1:F:64:PHE:CE2	1:F:68:LEU:HD11	2.46	0.50
1:F:831:GLU:HG3	1:F:840:TYR:CD1	2.45	0.50
1:F:845:ASN:HB3	1:F:848:GLU:HG2	1.93	0.50
1:A:29:ILE:CD1	1:A:152:PHE:CE1	2.94	0.50
1:A:474:LEU:HD11	1:A:538:ILE:HD11	1.92	0.50
1:A:751:ASN:CG	1:A:763:PRO:HG2	2.36	0.50
1:F:437:THR:O	1:F:439:GLU:N	2.44	0.50
1:F:640:LEU:HA	1:F:646:LYS:HD2	1.92	0.50
1:F:663:LEU:HD21	1:F:670:ILE:HG23	1.92	0.50
1:A:159:GLU:HG3	1:A:170:VAL:HG22	1.93	0.50
1:A:329:SER:O	1:A:333:LYS:HB2	2.11	0.50
1:F:159:GLU:HG3	1:F:170:VAL:HG22	1.93	0.50
1:F:288:TRP:CG	1:F:381:CYS:HB2	2.46	0.50
1:F:881:PRO:O	1:F:882:LEU:CB	2.60	0.50
1:F:900:ILE:HB	1:F:943:PHE:HB2	1.93	0.50
1:A:120:ILE:HG13	1:A:121:PHE:CD2	2.47	0.50
1:A:881:PRO:O	1:A:882:LEU:CB	2.60	0.50
1:F:143:GLY:H	7:F:1202:ANP:HNB1	1.59	0.50
1:F:776:ASP:O	1:F:777:ALA:O	2.29	0.50
1:F:936:GLN:O	1:F:942:LYS:HB3	2.10	0.50
1:A:276:ILE:HD12	1:A:277:PRO:CD	2.41	0.50
1:A:608:SER:O	1:A:609:LEU:C	2.54	0.50
1:A:143:GLY:H	7:A:1202:ANP:HNB1	1.59	0.50
1:A:776:ASP:O	1:A:777:ALA:O	2.29	0.50
1:A:159:GLU:HA	1:A:169:TYR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:ARG:HH12	1:F:356:LEU:HD11	1.77	0.50
1:A:490:LEU:HA	1:A:496:GLN:NE2	2.27	0.50
1:A:25:PRO:HB3	1:A:152:PHE:HZ	1.76	0.50
1:A:900:ILE:HB	1:A:943:PHE:HB2	1.93	0.50
1:F:148:LEU:O	1:F:152:PHE:HD2	1.95	0.50
1:F:159:GLU:HA	1:F:169:TYR:O	2.12	0.50
1:F:608:SER:O	1:F:609:LEU:C	2.54	0.50
2:G:2[A]:DC:H1'	2:G:3[A]:DT:H5'	1.92	0.50
1:A:96:GLU:CD	1:A:196:LYS:HE3	2.37	0.49
1:F:212:ASP:OD1	1:F:212:ASP:C	2.55	0.49
1:F:474:LEU:HD11	1:F:538:ILE:HD11	1.92	0.49
1:F:490:LEU:HA	1:F:496:GLN:NE2	2.27	0.49
1:A:231:ARG:HH12	1:A:356:LEU:HD11	1.77	0.49
1:F:723:GLN:C	1:F:726:PRO:HD2	2.37	0.49
1:A:64:PHE:CE2	1:A:68:LEU:HD11	2.46	0.49
1:F:643:SER:HB3	1:F:646:LYS:HG3	1.94	0.49
1:A:312:MET:HE1	1:F:369:GLN:OE1	2.12	0.49
1:A:530:ASP:O	1:A:534:ILE:HG12	2.12	0.49
2:B:11[A]:DC:N4	3:H:1[A]:DC:N4	2.60	0.49
1:F:96:GLU:CD	1:F:196:LYS:HE3	2.37	0.49
1:A:643:SER:HB3	1:A:646:LYS:HG3	1.94	0.49
1:F:436:GLY:HA3	1:F:517:ARG:HD2	1.93	0.49
1:A:571:PRO:HD3	1:A:596:THR:HG1	1.77	0.49
1:A:838:SER:HB3	5:E:10[B]:DT:H5'	1.94	0.49
1:A:326:LYS:O	1:A:330:GLU:HG3	2.13	0.49
1:F:326:LYS:O	1:F:330:GLU:HG3	2.13	0.49
1:F:562:PRO:HG3	1:F:579:TYR:HE1	1.78	0.49
1:F:646:LYS:O	1:F:649:ASP:HB2	2.13	0.49
1:F:883:ARG:O	1:F:884:TYR:CD1	2.66	0.49
1:A:369:GLN:OE1	1:F:312:MET:HE1	2.11	0.49
1:A:562:PRO:HG3	1:A:579:TYR:HE1	1.78	0.49
1:A:646:LYS:O	1:A:649:ASP:HB2	2.13	0.49
1:A:1044:PRO:HB3	1:F:1126:LYS:HE2	1.94	0.49
1:F:570:LYS:CB	1:F:596:THR:OG1	2.60	0.49
1:A:723:GLN:C	1:A:726:PRO:HD2	2.37	0.49
1:F:736:HIS:CG	2:G:10[A]:DA:H5''	2.47	0.49
1:A:212:ASP:OD1	1:A:212:ASP:C	2.55	0.48
1:A:845:ASN:HB3	1:A:848:GLU:HG2	1.94	0.48
1:A:1061:ASN:HB2	1:A:1108:GLU:OE2	2.13	0.48
1:F:120:ILE:HG13	1:F:121:PHE:CD2	2.47	0.48
1:F:482:ARG:C	1:F:483:GLU:HG2	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:C	1:A:483:GLU:HG2	2.37	0.48
1:F:490:LEU:HD23	1:F:490:LEU:O	2.13	0.48
1:A:734:TYR:CZ	1:A:736:HIS:HB2	2.48	0.48
1:F:734:TYR:CZ	1:F:736:HIS:HB2	2.48	0.48
1:F:752:PHE:CD1	1:F:753:VAL:O	2.65	0.48
1:A:883:ARG:O	1:A:884:TYR:CD1	2.66	0.48
1:F:25:PRO:HB3	1:F:152:PHE:HZ	1.76	0.48
1:F:530:ASP:O	1:F:534:ILE:HG12	2.13	0.48
1:F:1061:ASN:HB2	1:F:1108:GLU:OE2	2.13	0.48
5:J:12[B]:DA:H2''	5:J:13[B]:DT:O5'	2.13	0.48
1:A:119:MET:HE3	1:F:14:LYS:HB2	1.96	0.48
1:A:607:THR:HA	1:F:765:GLY:HA2	1.95	0.48
1:A:720:LYS:HD3	1:A:781:ARG:HA	1.96	0.48
1:A:752:PHE:CD1	1:A:753:VAL:O	2.65	0.48
1:A:490:LEU:HD23	1:A:490:LEU:O	2.13	0.48
1:A:736:HIS:CG	2:B:10[A]:DA:H5''	2.48	0.48
1:A:40:TRP:O	1:A:221:ARG:HD3	2.14	0.48
1:A:838:SER:HB3	3:C:10[A]:DA:H5'	1.95	0.48
1:F:720:LYS:HD3	1:F:781:ARG:HA	1.96	0.48
1:F:838:SER:HB3	3:H:10[A]:DA:H5'	1.94	0.48
1:F:571:PRO:CD	1:F:596:THR:HG1	2.27	0.48
3:H:14[A]:DG:H2''	3:H:15[A]:DG:OP2	2.14	0.48
1:F:74:ASN:CB	1:F:81:MET:HE1	2.30	0.47
1:F:329:SER:O	1:F:333:LYS:HB2	2.14	0.47
1:A:117:PRO:HB3	1:A:158:LEU:CD2	2.45	0.47
1:A:872:TRP:CH2	1:A:886:MET:HG3	2.49	0.47
1:A:850:ILE:HD11	1:A:1162:PHE:CE1	2.50	0.47
1:F:918:LEU:HD11	1:F:923:ASN:HB2	1.96	0.47
1:A:1005:TYR:CZ	1:A:1155:TRP:HA	2.50	0.47
1:F:95:ILE:HD13	1:F:219:MET:HE1	1.97	0.47
1:A:831:GLU:HG3	1:A:840:TYR:CD1	2.45	0.47
1:F:690:ARG:NH1	4:I:10[B]:DT:H4'	2.30	0.47
1:F:845:ASN:HB3	1:F:848:GLU:CG	2.45	0.47
5:E:12[B]:DA:H2''	5:E:13[B]:DT:O5'	2.14	0.47
1:F:117:PRO:HB3	1:F:158:LEU:CD2	2.45	0.47
1:F:399:ARG:CG	1:F:399:ARG:NH1	2.71	0.47
1:F:779:ALA:O	1:F:782[A]:PTR:HB3	2.14	0.47
1:F:1005:TYR:CZ	1:F:1155:TRP:HA	2.50	0.47
1:A:81:MET:HG3	1:A:100:ASP:OD1	2.15	0.47
1:A:806:ILE:O	1:A:813:VAL:HG22	2.15	0.47
1:A:845:ASN:HB3	1:A:848:GLU:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:TRP:CZ2	1:A:874:GLY:HA3	2.50	0.47
1:F:81:MET:HG3	1:F:100:ASP:OD1	2.15	0.47
1:F:852:ASN:ND2	1:F:865:MET:HE3	2.30	0.47
1:F:872:TRP:CZ2	1:F:874:GLY:HA3	2.50	0.47
1:A:14:LYS:HB2	1:F:119:MET:HE3	1.96	0.47
1:A:443:CYS:SG	1:A:468:TYR:HA	2.55	0.47
1:A:643:SER:O	1:A:644:LYS:C	2.58	0.47
1:A:810:GLU:O	1:A:810:GLU:HG2	2.15	0.47
1:A:852:ASN:ND2	1:A:865:MET:HE3	2.30	0.47
1:F:806:ILE:O	1:F:813:VAL:HG22	2.15	0.47
1:A:883:ARG:C	1:A:884:TYR:CD1	2.93	0.46
1:F:40:TRP:O	1:F:221:ARG:HD3	2.14	0.46
1:F:883:ARG:C	1:F:884:TYR:CD1	2.93	0.46
1:A:60:LEU:HD23	1:A:215:ILE:HG12	1.97	0.46
1:A:95:ILE:HD13	1:A:219:MET:HE1	1.97	0.46
1:A:1049:ILE:O	1:A:1053:GLU:HG2	2.15	0.46
1:F:1019:GLU:O	1:F:1023:TYR:HD2	1.98	0.46
1:F:1045:ARG:O	1:F:1049:ILE:HG13	2.16	0.46
4:I:2[B]:DG:N1	5:J:14[B]:DC:N3	2.63	0.46
1:A:242:LEU:O	1:A:243:LYS:HB2	2.15	0.46
1:A:765:GLY:HA2	1:F:607:THR:HA	1.98	0.46
1:A:918:LEU:HD11	1:A:923:ASN:HB2	1.97	0.46
1:F:872:TRP:CH2	1:F:886:MET:HG3	2.49	0.46
1:A:163:LEU:HD13	1:A:193:SER:HB3	1.98	0.46
1:A:1045:ARG:O	1:A:1049:ILE:HG13	2.16	0.46
1:F:443:CYS:SG	1:F:468:TYR:HA	2.55	0.46
1:F:850:ILE:HD11	1:F:1162:PHE:CE1	2.50	0.46
1:F:502:MET:SD	1:F:518:TYR:HB2	2.55	0.46
1:A:502:MET:SD	1:A:518:TYR:HB2	2.55	0.46
1:A:1139:LYS:HD3	1:A:1139:LYS:HA	1.80	0.46
1:F:1067:TYR:HE1	1:F:1070:SER:H	1.61	0.46
1:A:110:ASN:OD1	1:F:9:SER:HB3	2.15	0.46
1:A:1019:GLU:O	1:A:1023:TYR:HD2	1.98	0.46
1:F:60:LEU:HD23	1:F:215:ILE:HG12	1.97	0.46
1:F:242:LEU:O	1:F:243:LYS:HB2	2.15	0.46
1:F:1049:ILE:O	1:F:1053:GLU:HG2	2.15	0.46
1:F:630:LEU:HD23	1:F:672:ILE:HD12	1.98	0.46
1:F:657:TYR:CD2	1:F:657:TYR:C	2.93	0.46
1:F:810:GLU:O	1:F:810:GLU:HG2	2.15	0.46
1:F:850:ILE:HD11	1:F:1162:PHE:HE1	1.81	0.46
1:A:1126:LYS:HE2	1:F:1044:PRO:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:837:TRP:CD1	1:F:984:ILE:HD13	2.52	0.46
1:A:850:ILE:HD11	1:A:1162:PHE:HE1	1.81	0.45
1:A:1044:PRO:O	1:A:1046:ASN:N	2.49	0.45
1:F:365:GLN:O	1:F:367:LYS:HG3	2.16	0.45
1:F:643:SER:O	1:F:644:LYS:C	2.58	0.45
1:A:726:PRO:CG	1:F:726:PRO:HG2	2.46	0.45
1:A:767:PHE:CE2	1:A:783:ILE:HD12	2.52	0.45
1:A:901:THR:HA	1:A:941:ILE:O	2.17	0.45
1:F:512:ASP:CB	1:F:514:LYS:HG2	2.47	0.45
1:A:399:ARG:CG	1:A:399:ARG:NH1	2.71	0.45
1:A:837:TRP:CD1	1:A:984:ILE:HD13	2.51	0.45
1:A:800:ASP:HB2	1:A:801:PRO:HD3	1.99	0.45
1:F:29:ILE:CD1	1:F:152:PHE:CE1	2.94	0.45
1:A:337:LYS:C	1:A:338:LYS:HG3	2.42	0.45
1:F:533:HIS:HB2	1:F:683:PHE:CD2	2.52	0.45
1:A:1126:LYS:O	1:A:1130:GLN:HG2	2.17	0.45
1:F:667:LEU:O	1:F:668:LYS:HB3	2.17	0.45
1:F:706:VAL:HA	1:F:728:VAL:HG11	1.99	0.45
1:F:1044:PRO:O	1:F:1046:ASN:N	2.49	0.45
1:A:365:GLN:O	1:A:367:LYS:HG3	2.16	0.45
1:A:276:ILE:CD1	1:A:277:PRO:HD2	2.47	0.45
1:A:657:TYR:CD2	1:A:657:TYR:C	2.93	0.45
1:F:163:LEU:HD13	1:F:193:SER:HB3	1.98	0.45
1:F:562:PRO:HG3	1:F:579:TYR:CE1	2.52	0.45
1:A:29:ILE:CD1	1:A:152:PHE:CE2	2.61	0.45
1:A:533:HIS:HB2	1:A:683:PHE:CD2	2.52	0.45
1:A:592:SER:HB2	1:A:597:TRP:CE2	2.52	0.45
1:A:1107:GLU:HG2	1:A:1109:LEU:H	1.82	0.45
1:A:570:LYS:CB	1:A:596:THR:OG1	2.60	0.44
1:F:842:PRO:HG3	1:F:972:LEU:CD2	2.48	0.44
1:A:292:PHE:CZ	1:A:391:ILE:HG23	2.52	0.44
1:A:842:PRO:HG3	1:A:972:LEU:CD2	2.48	0.44
1:F:373:ARG:CZ	1:F:375:LYS:HE2	2.47	0.44
1:F:667:LEU:HD23	1:F:667:LEU:HA	1.82	0.44
1:F:800:ASP:HB2	1:F:801:PRO:HD3	1.99	0.44
1:F:1107:GLU:HG2	1:F:1109:LEU:H	1.82	0.44
1:A:373:ARG:CZ	1:A:375:LYS:HE2	2.47	0.44
1:A:706:VAL:HA	1:A:728:VAL:HG11	1.99	0.44
1:F:276:ILE:CD1	1:F:277:PRO:HD2	2.47	0.44
1:F:337:LYS:C	1:F:338:LYS:HG3	2.41	0.44
1:F:1126:LYS:O	1:F:1130:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:GLN:HG2	1:A:1143:LEU:HD21	2.00	0.44
1:F:292:PHE:CZ	1:F:391:ILE:HG23	2.52	0.44
1:F:901:THR:HA	1:F:941:ILE:O	2.17	0.44
1:A:630:LEU:HD23	1:A:672:ILE:HD12	1.98	0.44
1:A:1067:TYR:HE1	1:A:1070:SER:H	1.61	0.44
1:A:1069:GLY:O	1:A:1070:SER:HB3	2.18	0.44
1:F:762:LEU:HA	1:F:763:PRO:HD3	1.80	0.44
1:F:767:PHE:CE2	1:F:783:ILE:HD12	2.52	0.44
1:F:1001:ARG:HD2	1:F:1001:ARG:O	2.18	0.44
1:F:482:ARG:O	1:F:483:GLU:CB	2.66	0.44
1:F:543:GLU:HB2	1:F:550:LEU:HD12	2.00	0.44
1:A:895:ASP:O	1:A:896:ASN:HB2	2.17	0.44
1:A:1001:ARG:HA	1:A:1001:ARG:HD3	1.73	0.44
1:A:1115:TYR:CE2	1:A:1116:LEU:HG	2.53	0.44
1:F:592:SER:HB2	1:F:597:TRP:CE2	2.52	0.44
1:A:338:LYS:HB3	1:A:407:ASN:HB3	1.99	0.44
1:A:338:LYS:HB3	1:A:407:ASN:CB	2.47	0.44
1:A:667:LEU:O	1:A:668:LYS:HB3	2.17	0.44
1:A:1001:ARG:HD2	1:A:1001:ARG:O	2.18	0.44
2:B:11[A]:DC:C4	3:H:1[A]:DC:C4	3.06	0.44
1:A:276:ILE:HA	1:A:277:PRO:HD3	1.84	0.44
1:F:276:ILE:HA	1:F:277:PRO:HD3	1.84	0.44
1:F:287:ARG:HH12	1:F:358:GLU:HG3	1.83	0.44
1:F:292:PHE:CE2	1:F:391:ILE:HG23	2.53	0.44
1:F:580:ASN:ND2	1:F:582:PRO:HD2	2.33	0.44
1:F:895:ASP:O	1:F:896:ASN:HB2	2.17	0.44
1:F:1069:GLY:O	1:F:1070:SER:HB3	2.18	0.44
1:A:512:ASP:CB	1:A:514:LYS:HG2	2.47	0.43
1:A:1029:PHE:CZ	1:A:1033:ILE:HD11	2.53	0.43
1:F:74:ASN:HD22	1:F:99:ASN:ND2	2.16	0.43
1:F:1029:PHE:CZ	1:F:1033:ILE:HD11	2.53	0.43
1:A:9:SER:HB3	1:F:110:ASN:OD1	2.18	0.43
1:A:437:THR:CG2	1:A:438:LYS:N	2.65	0.43
1:A:74:ASN:HD22	1:A:99:ASN:ND2	2.16	0.43
1:A:361:ALA:O	1:A:370:LEU:HD12	2.19	0.43
1:A:543:GLU:HB2	1:A:550:LEU:HD12	1.99	0.43
1:F:896:ASN:HD21	1:F:949:PRO:HG3	1.83	0.43
1:F:1017:GLN:HG2	1:F:1143:LEU:HD21	2.00	0.43
1:A:405:ASP:OD1	1:A:405:ASP:O	2.37	0.43
1:A:287:ARG:HH12	1:A:358:GLU:HG3	1.83	0.43
1:A:297:ILE:O	1:F:341:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASN:ND2	1:A:582:PRO:HD2	2.33	0.43
1:A:1005:TYR:CE2	1:A:1155:TRP:CG	3.07	0.43
3:C:2[A]:DG:N2	3:H:3[A]:DC:N3	2.66	0.43
1:F:525:THR:O	1:F:527:GLN:N	2.52	0.43
1:A:75:LYS:HE2	1:A:231:ARG:O	2.19	0.43
1:A:562:PRO:HG3	1:A:579:TYR:CE1	2.52	0.43
1:A:570:LYS:N	1:A:571:PRO:HD2	2.34	0.43
1:A:899:GLU:HA	1:A:943:PHE:O	2.19	0.43
1:F:769:THR:N	1:F:776:ASP:OD2	2.52	0.43
1:A:769:THR:N	1:A:776:ASP:OD2	2.52	0.43
1:F:75:LYS:HE2	1:F:231:ARG:O	2.19	0.43
1:F:1007:LYS:HB2	1:F:1007:LYS:HE3	1.82	0.43
1:F:1026:GLN:O	1:F:1030:ILE:HG12	2.19	0.43
1:A:451:ASP:HA	1:A:454:LEU:HB3	2.00	0.43
1:A:726:PRO:HG2	1:F:726:PRO:CG	2.46	0.43
1:A:896:ASN:HD21	1:A:949:PRO:HG3	1.83	0.43
1:A:969:PRO:HG2	3:C:12[A]:DT:H5''	2.00	0.43
1:F:1005:TYR:CE2	1:F:1155:TRP:CG	3.07	0.43
1:A:726:PRO:HB3	1:F:723:GLN:HA	2.00	0.43
1:A:292:PHE:CE2	1:A:391:ILE:HG23	2.53	0.42
1:A:598:LYS:HD3	1:A:599:GLN:N	2.34	0.42
1:F:779:ALA:H	1:F:782[A]:PTR:HD1	1.83	0.42
1:A:29:ILE:HD13	1:A:152:PHE:CD2	2.43	0.42
1:A:398:THR:HG22	1:F:490:LEU:HD21	2.01	0.42
1:A:723:GLN:HA	1:F:726:PRO:HB3	2.01	0.42
1:A:1042:ASN:HB3	1:A:1043:LYS:H	1.68	0.42
1:F:570:LYS:N	1:F:571:PRO:HD2	2.34	0.42
1:F:1115:TYR:CE2	1:F:1116:LEU:HG	2.53	0.42
1:A:482:ARG:O	1:A:483:GLU:CB	2.66	0.42
1:A:667:LEU:HD23	1:A:667:LEU:HA	1.82	0.42
1:F:147:LYS:O	1:F:151:ILE:HG13	2.20	0.42
1:F:598:LYS:HD3	1:F:599:GLN:N	2.34	0.42
1:F:361:ALA:O	1:F:370:LEU:HD12	2.19	0.42
1:F:674:ASP:O	1:F:678:LYS:HB2	2.19	0.42
1:A:313:GLY:O	1:A:369:GLN:HA	2.20	0.42
1:A:674:ASP:O	1:A:678:LYS:HB2	2.19	0.42
2:B:2[A]:DC:H1'	2:B:3[A]:DT:H5'	2.01	0.42
1:F:426:TYR:CZ	1:F:497:ALA:HA	2.55	0.42
1:F:451:ASP:HA	1:F:454:LEU:HB3	2.00	0.42
1:F:613:VAL:O	1:F:616:TYR:HB2	2.20	0.42
1:A:115:TYR:HB3	1:A:117:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD21	1:A:350:PHE:CD1	2.55	0.42
1:A:335:LYS:NZ	2:G:4[A]:DA:OP1	2.53	0.42
1:A:449:GLU:OE1	1:A:526:ASP:CG	2.62	0.42
1:F:231:ARG:HH22	1:F:356:LEU:HD11	1.85	0.42
1:A:525:THR:O	1:A:527:GLN:N	2.52	0.42
1:A:1026:GLN:O	1:A:1030:ILE:HG12	2.19	0.42
1:F:92:GLU:O	1:F:93:HIS:C	2.62	0.42
1:F:899:GLU:HA	1:F:943:PHE:O	2.19	0.42
1:A:147:LYS:O	1:A:151:ILE:HG13	2.20	0.42
1:A:829:GLY:HA3	1:A:841:ILE:O	2.20	0.42
1:F:870:ARG:HE	1:F:1173:ASP:CG	2.28	0.42
1:F:910:SER:O	1:F:914:GLU:HG3	2.20	0.42
1:F:949:PRO:O	1:F:952:MET:HB2	2.20	0.42
1:A:580:ASN:HB2	1:A:582:PRO:HD2	2.02	0.42
1:A:968:SER:HA	1:A:969:PRO:HD3	1.83	0.42
3:C:3[A]:DC:N3	3:H:2[A]:DG:N2	2.68	0.42
1:A:93:HIS:CE1	1:A:210:GLU:HA	2.55	0.42
1:A:95:ILE:CD1	1:A:219:MET:HE1	2.50	0.42
1:A:426:TYR:CZ	1:A:497:ALA:HA	2.55	0.42
1:A:1041:THR:CG2	1:F:1034:ILE:HG12	2.50	0.42
2:B:4[A]:DA:OP1	1:F:335:LYS:NZ	2.52	0.42
1:F:95:ILE:CD1	1:F:219:MET:HE1	2.50	0.42
1:A:231:ARG:HH22	1:A:356:LEU:HD11	1.85	0.41
1:A:341:LYS:HE2	1:F:297:ILE:O	2.20	0.41
1:A:646:LYS:HB3	1:A:649:ASP:HB2	2.02	0.41
1:A:819:LEU:HD21	1:A:1001:ARG:HA	2.02	0.41
1:A:1034:ILE:HG12	1:F:1041:THR:CG2	2.50	0.41
1:F:93:HIS:CE1	1:F:210:GLU:HA	2.55	0.41
1:F:313:GLY:O	1:F:369:GLN:HA	2.20	0.41
1:A:136:LYS:HE3	1:A:136:LYS:HB2	1.88	0.41
1:A:613:VAL:O	1:A:616:TYR:HB2	2.20	0.41
1:A:799:ASP:CG	1:A:1001:ARG:HH22	2.29	0.41
1:A:1041:THR:O	1:A:1042:ASN:HB2	2.20	0.41
1:F:41:ILE:HG22	1:F:42:TYR:N	2.35	0.41
1:F:423:ILE:HD11	1:F:517:ARG:NH2	2.35	0.41
1:F:1041:THR:O	1:F:1042:ASN:HB2	2.20	0.41
1:A:949:PRO:O	1:A:952:MET:HB2	2.20	0.41
1:F:115:TYR:HB3	1:F:117:PRO:HD2	2.02	0.41
1:F:340:VAL:CG1	1:F:344:GLN:OE1	2.68	0.41
1:F:969:PRO:HG2	3:H:12[A]:DT:H5"	2.02	0.41
1:F:1034:ILE:C	1:F:1036:LYS:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:HIS:HA	1:A:797:PRO:HD3	1.91	0.41
1:F:1010:ASP:O	1:F:1013:SER:HB2	2.20	0.41
1:A:476:GLY:O	1:A:477:LYS:C	2.63	0.41
1:F:141:ARG:HD3	1:F:360:PRO:HD2	2.03	0.41
1:F:333:LYS:CG	1:F:339:SER:HB3	2.38	0.41
1:F:690:ARG:NH1	2:G:10[A]:DA:H4'	2.36	0.41
1:F:769:THR:HG23	1:F:776:ASP:OD2	2.20	0.41
1:F:819:LEU:HD21	1:F:1001:ARG:HA	2.02	0.41
1:A:581:MET:N	1:A:582:PRO:CD	2.83	0.41
1:A:814:GLU:HG2	1:A:815:PRO:O	2.20	0.41
1:A:870:ARG:HE	1:A:1173:ASP:CG	2.28	0.41
1:F:546:PHE:HA	1:F:547:PRO:HD2	1.95	0.41
1:F:700:LYS:O	1:F:701:PRO:C	2.63	0.41
1:F:752:PHE:C	1:F:753:VAL:O	2.61	0.41
1:F:799:ASP:CG	1:F:1001:ARG:HH22	2.28	0.41
1:F:814:GLU:HG2	1:F:815:PRO:O	2.20	0.41
1:A:92:GLU:O	1:A:93:HIS:C	2.62	0.41
1:A:482:ARG:O	1:A:483:GLU:HB2	2.20	0.41
1:A:490:LEU:HD21	1:F:398:THR:HG22	2.03	0.41
1:A:700:LYS:O	1:A:701:PRO:C	2.63	0.41
1:A:769:THR:HG23	1:A:776:ASP:OD2	2.20	0.41
1:A:1041:THR:HG21	1:F:1034:ILE:HA	2.03	0.41
1:F:482:ARG:O	1:F:483:GLU:HB2	2.20	0.41
1:F:580:ASN:HB2	1:F:582:PRO:HD2	2.02	0.41
1:F:647:ALA:HA	1:F:650:ARG:NH1	2.36	0.41
1:A:910:SER:O	1:A:914:GLU:HG3	2.20	0.41
1:A:1010:ASP:O	1:A:1013:SER:HB2	2.20	0.41
1:F:90:ALA:O	1:F:93:HIS:HD2	2.04	0.41
1:F:423:ILE:CD1	1:F:517:ARG:HH22	2.34	0.41
1:F:581:MET:N	1:F:582:PRO:CD	2.83	0.41
1:F:1070:SER:O	1:F:1070:SER:OG	2.30	0.41
1:A:41:ILE:HG22	1:A:42:TYR:N	2.35	0.41
1:A:90:ALA:O	1:A:93:HIS:HD2	2.04	0.41
1:A:1026:GLN:HA	1:A:1116:LEU:CD2	2.51	0.41
1:A:1067:TYR:HE1	1:A:1070:SER:N	2.18	0.41
1:F:258:LEU:HD21	1:F:350:PHE:CD1	2.55	0.41
1:F:720:LYS:HB3	1:F:784:TYR:CE2	2.56	0.41
1:F:829:GLY:HA3	1:F:841:ILE:O	2.20	0.41
4:I:1[B]:DG:N1	5:J:15[B]:DC:N3	2.69	0.41
1:A:423:ILE:CD1	1:A:517:ARG:HH22	2.34	0.41
1:A:851:LYS:HA	1:A:854:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:646:LYS:HB3	1:F:649:ASP:HB2	2.02	0.41
1:F:837:TRP:CG	1:F:984:ILE:HD13	2.56	0.41
1:F:851:LYS:HA	1:F:854:ARG:NH2	2.36	0.41
1:F:931:LYS:HB3	1:F:946:THR:O	2.21	0.41
1:F:1026:GLN:HA	1:F:1116:LEU:CD2	2.51	0.41
1:F:1065:LYS:HA	1:F:1066:PRO:HD3	1.77	0.41
1:A:124:LEU:HD21	1:A:151:ILE:HD11	2.03	0.40
1:A:762:LEU:HA	1:A:763:PRO:HD3	1.80	0.40
1:A:1034:ILE:C	1:A:1036:LYS:H	2.29	0.40
1:A:1053:GLU:HB3	1:A:1113:TYR:OH	2.21	0.40
1:A:1123:SER:HA	1:A:1128:ARG:CB	2.51	0.40
1:F:476:GLY:O	1:F:477:LYS:C	2.63	0.40
1:A:333:LYS:CG	1:A:339:SER:HB3	2.38	0.40
1:A:396:LEU:HD23	1:A:396:LEU:C	2.47	0.40
1:A:423:ILE:HD11	1:A:517:ARG:NH2	2.35	0.40
1:A:668:LYS:O	1:A:668:LYS:CG	2.67	0.40
1:A:723:GLN:O	1:A:726:PRO:HD2	2.22	0.40
1:A:1040:VAL:HG13	1:A:1048:ILE:CD1	2.51	0.40
1:A:1047:ALA:O	1:A:1051:GLU:HG3	2.22	0.40
1:F:434:LYS:HD3	1:F:439:GLU:OE1	2.21	0.40
2:G:10[A]:DA:H2'	2:G:11[A]:DC:H6	1.87	0.40
1:A:879:ILE:HG22	1:A:880:GLU:HG3	2.04	0.40
1:A:994:LEU:HD23	1:A:994:LEU:C	2.46	0.40
1:A:1117:LEU:O	1:F:1121:ILE:HB	2.21	0.40
1:F:664:ASP:HB3	1:F:667:LEU:HG	2.03	0.40
1:A:454:LEU:O	1:A:458:VAL:HG13	2.22	0.40
5:E:3[B]:DC:N3	5:J:2[B]:DG:N1	2.69	0.40
1:F:769:THR:H	1:F:776:ASP:CG	2.30	0.40
1:F:879:ILE:HG22	1:F:880:GLU:HG3	2.04	0.40
1:A:338:LYS:O	1:A:339:SER:C	2.64	0.40
1:A:434:LYS:HD3	1:A:439:GLU:OE1	2.21	0.40
1:A:571:PRO:CD	1:A:596:THR:HG1	2.35	0.40
1:A:664:ASP:HA	1:A:665:PRO:HD3	1.93	0.40
1:A:979:ASP:HB2	1:A:980:PRO:CD	2.52	0.40
1:A:1034:ILE:HA	1:F:1041:THR:HG21	2.04	0.40
2:B:6[A]:DT:H6	2:B:6[A]:DT:H2'	1.73	0.40
1:F:437:THR:CG2	1:F:438:LYS:N	2.65	0.40
1:F:707:LEU:HD23	1:F:707:LEU:HA	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1091/1178 (93%)	1038 (95%)	52 (5%)	1 (0%)	48	83
1	F	1087/1178 (92%)	1034 (95%)	52 (5%)	1 (0%)	48	83
All	All	2178/2356 (92%)	2072 (95%)	104 (5%)	2 (0%)	48	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	ASP
1	F	526	ASP

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	992/1055 (94%)	985 (99%)	7 (1%)	76	79
1	F	989/1055 (94%)	982 (99%)	7 (1%)	76	79
All	All	1981/2110 (94%)	1967 (99%)	14 (1%)	76	79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	200	LYS
1	A	333	LYS
1	A	399	ARG

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Mol	Chain	Res	Type
1	A	402	GLU
1	A	883	ARG
1	A	1001	ARG
1	F	51	GLU
1	F	200	LYS
1	F	333	LYS
1	F	399	ARG
1	F	402	GLU
1	F	883	ARG
1	F	1001	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	74	ASN
1	A	167	GLN
1	A	176	ASN
1	A	227	ASN
1	A	348	ASN
1	A	593	HIS
1	A	619	ASN
1	A	858	ASN
1	A	1026	GLN
1	A	1050	GLN
1	A	1167	GLN
1	F	17	GLN
1	F	74	ASN
1	F	142	ASN
1	F	167	GLN
1	F	227	ASN
1	F	348	ASN
1	F	593	HIS
1	F	619	ASN
1	F	736	HIS
1	F	858	ASN
1	F	1026	GLN
1	F	1167	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PTR	F	782[A]	1	15,16,17	2.03	1 (6%)	17,22,24	0.61	0
1	PTR	A	782[A]	1	15,16,17	2.03	1 (6%)	17,22,24	0.60	0
4	TSP	I	11[B]	4	17,21,22	3.30	6 (35%)	21,30,33	2.57	7 (33%)
4	TSP	D	11[B]	4	17,21,22	3.30	6 (35%)	21,30,33	2.50	7 (33%)

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
1	PTR	F	782[A]	1	-	2/10/11/13	0/1/1/1
1	PTR	A	782[A]	1	-	2/10/11/13	0/1/1/1
4	TSP	I	11[B]	4	-	2/7/21/22	0/2/2/2
4	TSP	D	11[B]	4	-	2/7/21/22	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	782[A]	PTR	OH-CZ	-7.69	1.23	1.40
1	A	782[A]	PTR	OH-CZ	-7.65	1.23	1.40
4	I	11[B]	TSP	O4-C4	7.10	1.37	1.23
4	D	11[B]	TSP	O4-C4	7.06	1.37	1.23
4	I	11[B]	TSP	C2'-C3'	-6.15	1.36	1.52
4	D	11[B]	TSP	C2'-C3'	-6.09	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	11[B]	TSP	C4-C5	-5.61	1.35	1.44
4	D	11[B]	TSP	C4-C5	-5.52	1.35	1.44
4	D	11[B]	TSP	C6-C5	4.94	1.42	1.34
4	I	11[B]	TSP	C6-C5	4.89	1.42	1.34
4	D	11[B]	TSP	O5'-C5'	-3.67	1.33	1.44
4	I	11[B]	TSP	O5'-C5'	-3.54	1.33	1.44
4	D	11[B]	TSP	O4'-C4'	-3.29	1.37	1.45
4	I	11[B]	TSP	O4'-C4'	-3.24	1.37	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	11[B]	TSP	C5-C4-N3	5.68	120.26	115.32
4	D	11[B]	TSP	C5-C4-N3	5.52	120.12	115.32
4	I	11[B]	TSP	C4-N3-C2	-5.41	120.25	127.34
4	D	11[B]	TSP	C4-N3-C2	-5.33	120.36	127.34
4	I	11[B]	TSP	O4-C4-C5	-4.85	119.37	124.92
4	D	11[B]	TSP	O4-C4-C5	-4.76	119.47	124.92
4	I	11[B]	TSP	N3-C2-N1	3.75	119.77	114.89
4	D	11[B]	TSP	N3-C2-N1	3.71	119.72	114.89
4	D	11[B]	TSP	C5-C6-N1	-3.24	119.79	123.31
4	I	11[B]	TSP	C5-C6-N1	-3.10	119.94	123.31
4	D	11[B]	TSP	C6-C5-C4	2.39	119.99	118.02
4	I	11[B]	TSP	C6-C5-C4	2.20	119.84	118.02
4	I	11[B]	TSP	C5M-C5-C6	-2.14	119.95	122.85
4	D	11[B]	TSP	C5M-C5-C6	-2.01	120.14	122.85

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	11[B]	TSP	O4'-C4'-C5'-O5'
4	I	11[B]	TSP	O4'-C4'-C5'-O5'
4	I	11[B]	TSP	C3'-C4'-C5'-O5'
4	D	11[B]	TSP	C3'-C4'-C5'-O5'
1	F	782[A]	PTR	CA-CB-CG-CD2
1	F	782[A]	PTR	CA-CB-CG-CD1
1	A	782[A]	PTR	CA-CB-CG-CD2
1	A	782[A]	PTR	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	782[A]	PTR	6	0
1	A	782[A]	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
7	ANP	A	1202	6	33,33,33	1.71	10 (30%)	45,52,52	1.78	9 (20%)
7	ANP	F	1202	6	33,33,33	1.72	10 (30%)	45,52,52	1.77	9 (20%)

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
7	ANP	A	1202	6	-	4/18/38/38	0/3/3/3
7	ANP	F	1202	6	-	4/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1202	ANP	C6-N6	3.73	1.43	1.34
7	F	1202	ANP	C6-N6	3.71	1.43	1.34
7	A	1202	ANP	C5-C4	3.06	1.44	1.39
7	F	1202	ANP	C5-C4	3.02	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	1202	ANP	PG-O3G	-2.55	1.50	1.56
7	A	1202	ANP	PG-O3G	-2.54	1.50	1.56
7	F	1202	ANP	PB-O1B	2.52	1.50	1.46
7	A	1202	ANP	PB-O1B	2.51	1.50	1.46
7	A	1202	ANP	PG-O2G	-2.50	1.50	1.56
7	F	1202	ANP	PG-O2G	-2.50	1.50	1.56
7	F	1202	ANP	PB-O2B	-2.43	1.50	1.56
7	F	1202	ANP	O4'-C4'	-2.42	1.39	1.45
7	A	1202	ANP	PB-O2B	-2.42	1.50	1.56
7	F	1202	ANP	C8-N7	2.40	1.36	1.31
7	A	1202	ANP	O4'-C4'	-2.39	1.39	1.45
7	A	1202	ANP	C8-N7	2.38	1.36	1.31
7	F	1202	ANP	PG-O1G	2.32	1.49	1.46
7	A	1202	ANP	PG-O1G	2.29	1.49	1.46
7	F	1202	ANP	O3'-C3'	-2.23	1.37	1.43
7	A	1202	ANP	O3'-C3'	-2.21	1.37	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1202	ANP	C5-C4-N3	-5.30	119.42	126.72
7	F	1202	ANP	C5-C4-N3	-5.30	119.42	126.72
7	A	1202	ANP	N3-C4-N9	4.44	134.72	127.17
7	F	1202	ANP	N3-C4-N9	4.41	134.67	127.17
7	A	1202	ANP	N3-C2-N1	-3.58	123.16	128.58
7	F	1202	ANP	N3-C2-N1	-3.55	123.21	128.58
7	A	1202	ANP	C2-N3-C4	3.54	120.48	111.83
7	F	1202	ANP	C2-N3-C4	3.52	120.43	111.83
7	A	1202	ANP	C3'-C2'-C1'	2.85	106.85	101.46
7	F	1202	ANP	C3'-C2'-C1'	2.84	106.84	101.46
7	A	1202	ANP	C4-N9-C8	2.77	108.65	105.74
7	F	1202	ANP	C4-N9-C8	2.75	108.63	105.74
7	F	1202	ANP	C4-C5-N7	-2.41	107.82	110.58
7	A	1202	ANP	C4-C5-N7	-2.40	107.83	110.58
7	A	1202	ANP	N9-C8-N7	-2.30	110.68	113.94
7	F	1202	ANP	N9-C8-N7	-2.29	110.68	113.94
7	A	1202	ANP	C5-N7-C8	2.25	106.98	103.45
7	F	1202	ANP	C5-N7-C8	2.24	106.96	103.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

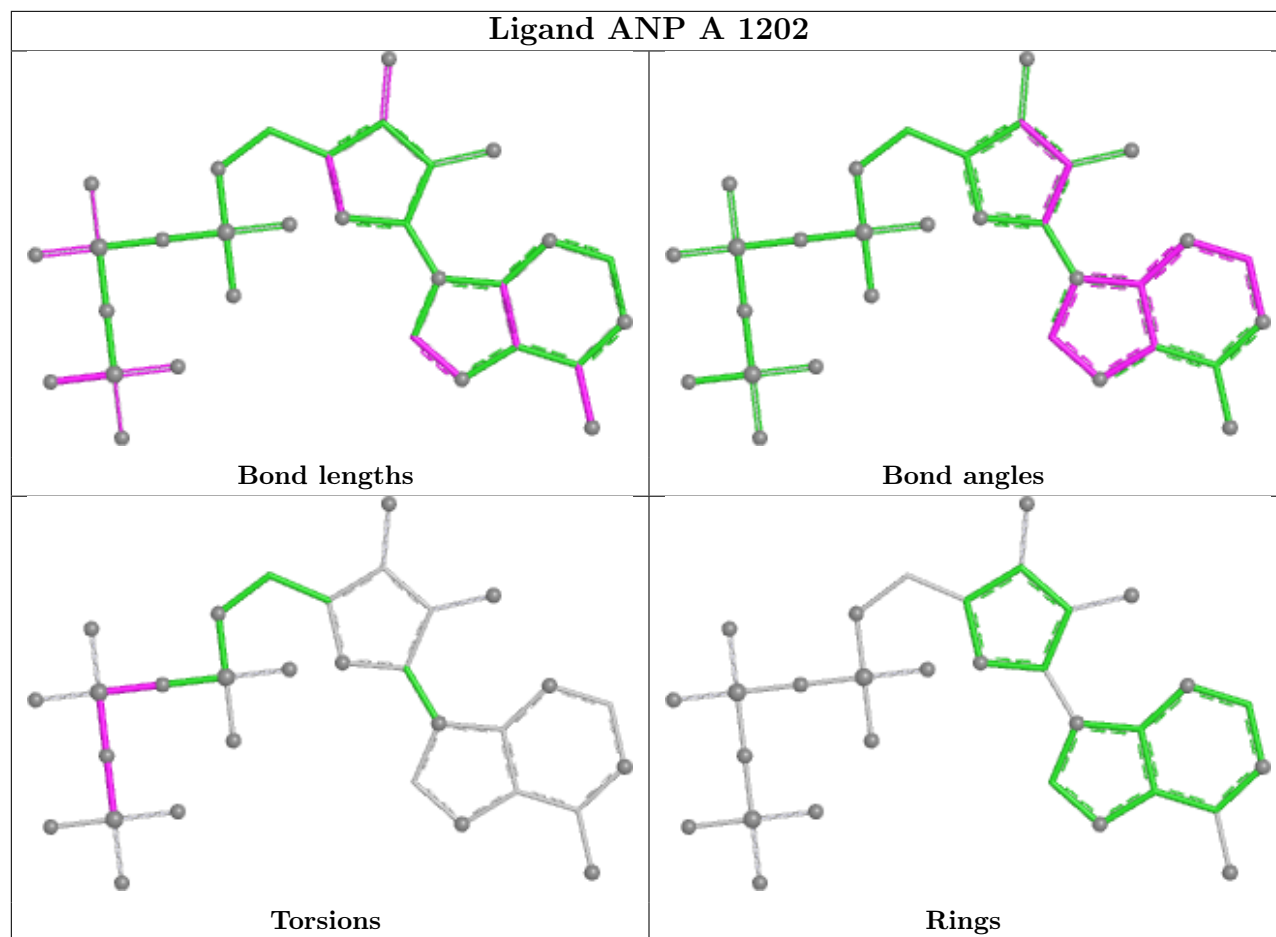
Mol	Chain	Res	Type	Atoms
7	A	1202	ANP	PB-N3B-PG-O1G
7	A	1202	ANP	PA-O3A-PB-O2B
7	F	1202	ANP	PB-N3B-PG-O1G
7	F	1202	ANP	PA-O3A-PB-O2B
7	A	1202	ANP	PA-O3A-PB-O1B
7	F	1202	ANP	PA-O3A-PB-O1B
7	A	1202	ANP	PG-N3B-PB-O3A
7	F	1202	ANP	PG-N3B-PB-O3A

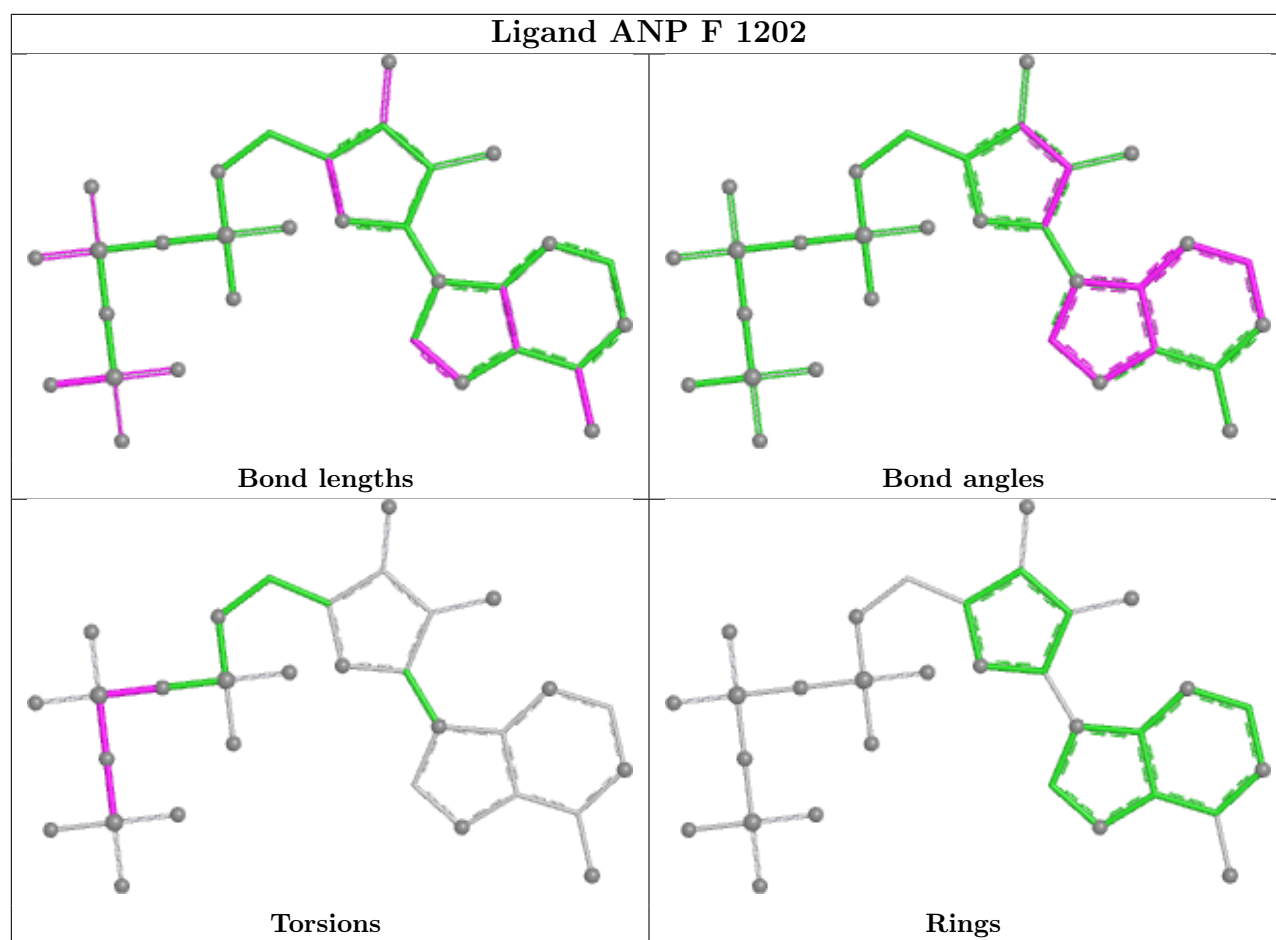
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1202	ANP	2	0
7	F	1202	ANP	2	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	1101/1178 (93%)	-0.07	28 (2%) 58 45	150, 238, 317, 403	0
1	F	1097/1178 (93%)	-0.07	27 (2%) 58 45	146, 240, 314, 414	0
2	B	11/11 (100%)	0.58	0 100 100	87, 134, 174, 182	11 (100%)
2	G	11/11 (100%)	0.69	0 100 100	79, 113, 165, 166	11 (100%)
3	C	15/15 (100%)	0.83	1 (6%) 24 25	108, 136, 213, 215	15 (100%)
3	H	15/15 (100%)	0.57	1 (6%) 24 25	101, 132, 188, 216	15 (100%)
4	D	10/11 (90%)	0.61	0 100 100	82, 122, 182, 214	10 (100%)
4	I	10/11 (90%)	0.83	0 100 100	84, 137, 201, 209	10 (100%)
5	E	15/15 (100%)	0.74	1 (6%) 24 25	81, 127, 180, 191	15 (100%)
5	J	15/15 (100%)	0.51	1 (6%) 24 25	90, 146, 166, 188	15 (100%)
All	All	2300/2460 (93%)	-0.03	59 (2%) 57 44	79, 236, 315, 414	102 (4%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	ASN	5.9
1	A	13	GLN	5.8
1	F	182	PRO	5.0
1	F	563	ILE	4.8
1	A	180	CYS	4.2
1	A	421	SER	4.1
1	F	10	ASP	4.1
1	A	10	ASP	4.0
1	F	500	LYS	4.0
1	A	438	LYS	3.8
1	F	421	SER	3.5
1	F	436	GLY	3.4
1	A	592	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	717	SER	3.2
1	F	173	TRP	3.2
1	A	667	LEU	3.1
1	A	596	THR	3.1
1	F	175	ASN	3.0
3	H	13[A]	DA	2.9
1	A	110	ASN	2.8
1	F	181	HIS	2.7
1	A	131	ASP	2.7
1	A	775	LYS	2.7
1	F	564	ILE	2.7
1	A	171	GLN	2.7
1	F	110	ASN	2.6
1	A	953	ALA	2.6
1	F	971	SER	2.5
1	F	956	ARG	2.5
1	A	563	ILE	2.5
1	A	434	LYS	2.4
3	C	13[A]	DA	2.4
1	A	842	PRO	2.4
1	F	13	GLN	2.4
1	A	830	ALA	2.4
1	F	278	THR	2.3
1	A	571	PRO	2.3
1	A	956	ARG	2.3
1	F	437	THR	2.3
1	F	577	ALA	2.3
1	F	631	GLN	2.3
1	A	27	THR	2.3
1	A	154	THR	2.3
1	F	171	GLN	2.3
1	F	842	PRO	2.2
1	A	111	LYS	2.2
1	A	173	TRP	2.2
1	F	889	ARG	2.2
1	A	37	GLN	2.1
1	A	664	ASP	2.1
1	A	181	HIS	2.1
5	E	13[B]	DT	2.1
1	F	666	THR	2.1
1	F	867	PRO	2.1
1	F	578	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
5	J	13[B]	DT	2.0
1	F	27	THR	2.0
1	F	168	LYS	2.0
1	A	666	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	A	782[A]	16/17	0.92	0.14	281,285,288,289	16
1	PTR	F	782[A]	16/17	0.96	0.16	299,305,310,312	16
4	TSP	D	11[B]	20/21	0.97	0.13	501,508,514,517	20
4	TSP	I	11[B]	20/21	0.99	0.13	429,437,440,441	20

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

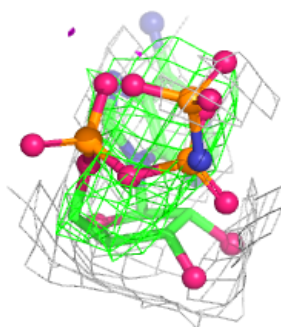
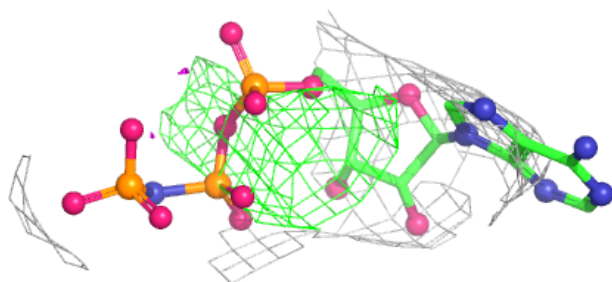
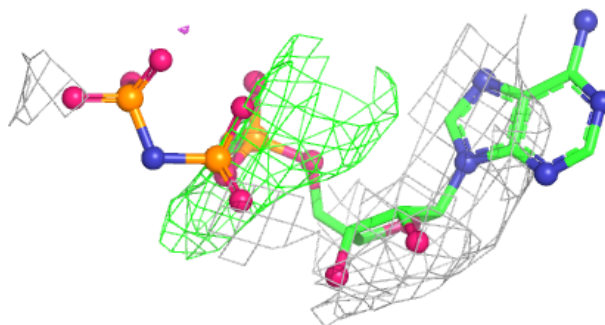
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	A	1201	1/1	0.98	0.05	115,115,115,115	0
6	MG	F	1201	1/1	0.98	0.05	114,114,114,114	0
7	ANP	A	1202	31/31	0.98	0.08	230,235,236,237	0
7	ANP	F	1202	31/31	0.99	0.07	229,235,247,251	0

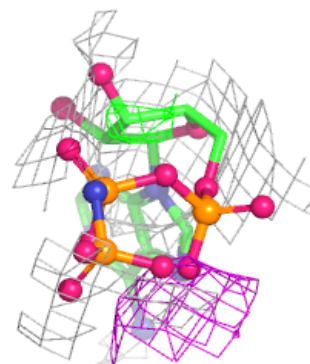
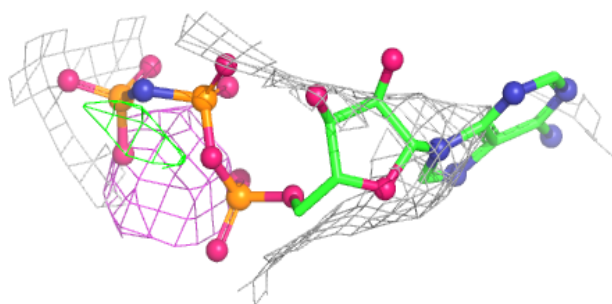
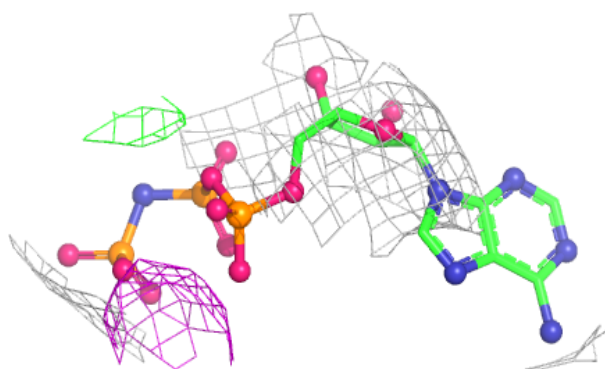
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ANP A 1202:

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

**Electron density around ANP F 1202:**

$2mF_o-DF_c$ (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.