



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:32 AM UTC

PDB ID : 4Z1I / pdb_00004z1i
Title : Crystal structure of human Trap1 with AMPPNP
Authors : Lee, C.; Park, H.K.; Ryu, J.H.; Kang, B.H.
Deposited on : 2015-03-27
Resolution : 3.30 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

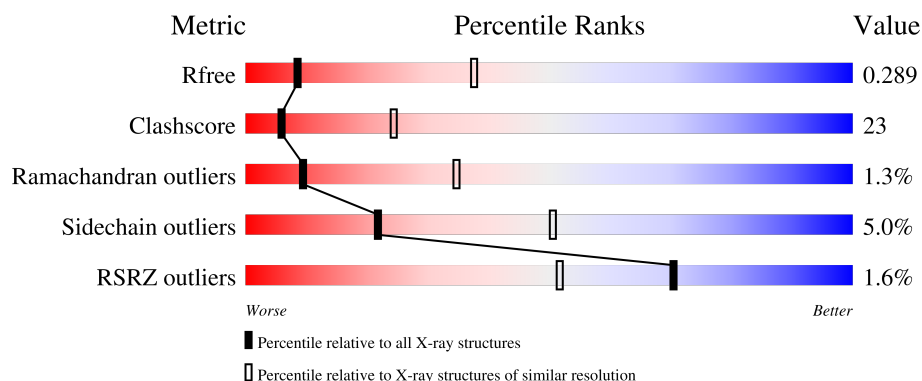
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	502	2% 42% 26% . . 27%
1	B	502	62% 27% . . 6%
1	C	502	57% 31% 5% . 6%
1	D	502	2% 56% 27% 5% . 11%

2 Entry composition [i](#)

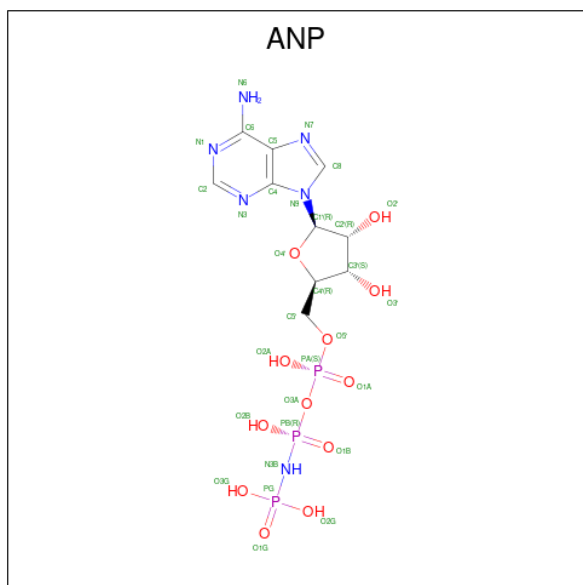
There are 3 unique types of molecules in this entry. The entry contains 14236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heat shock protein 75 kDa, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2911	1855	499	547	10			
1	B	472	Total	C	N	O	S	0	0	0
			3798	2417	648	719	14			
1	C	471	Total	C	N	O	S	0	0	0
			3787	2409	647	718	13			
1	D	449	Total	C	N	O	S	0	0	0
			3612	2303	614	682	13			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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

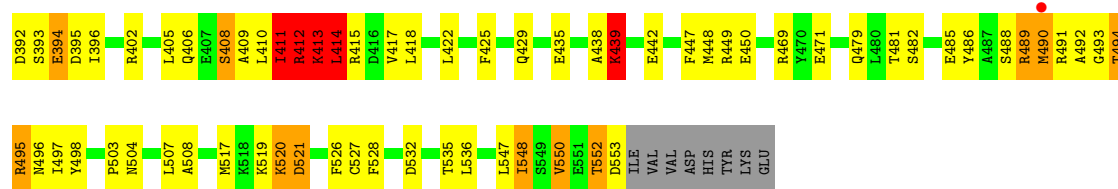
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

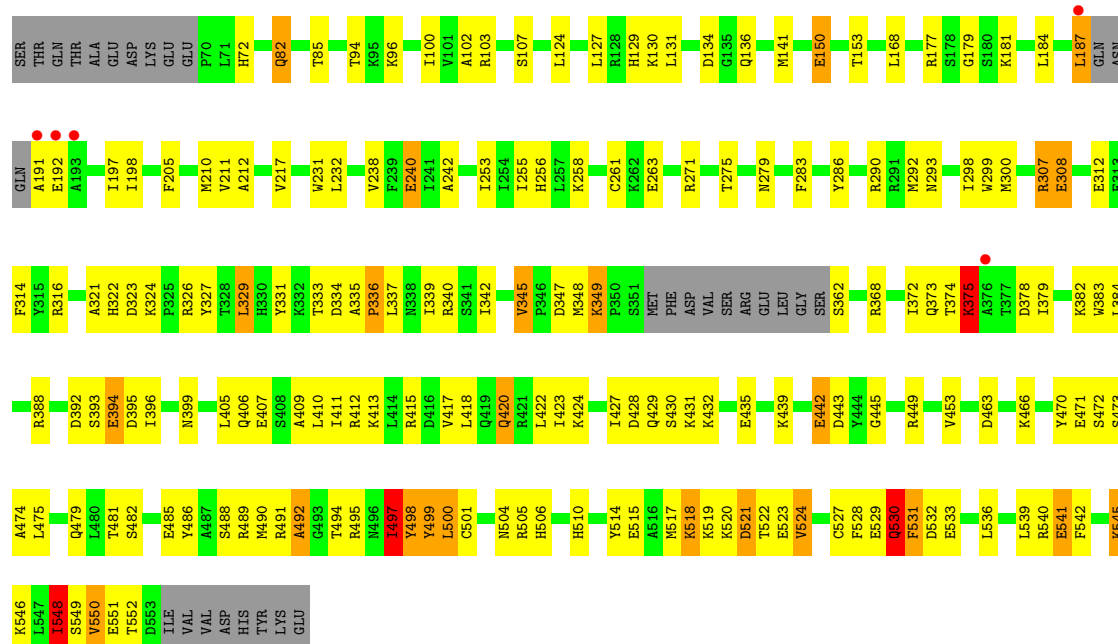
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- [illegible]

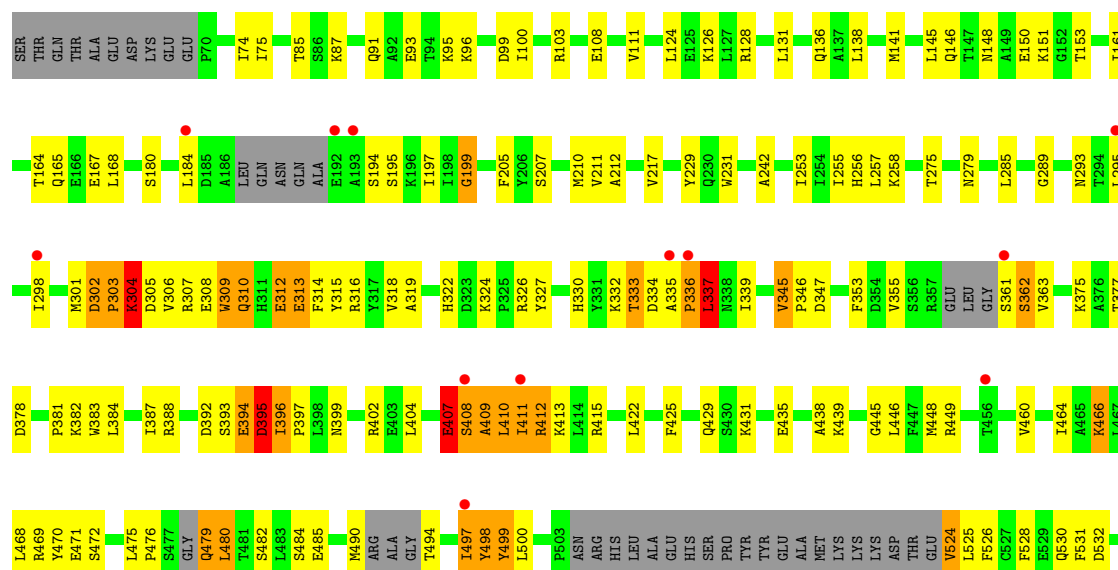
- Chain B:
-
- | Amino Acid | Count | Color |
|------------|-------|-------|
| SER | 1 | Grey |
| THR | 1 | Grey |
| GLN | 1 | Grey |
| THR | 1 | Grey |
| ALA | 1 | Grey |
| GLU | 1 | Grey |
| ASP | 1 | Grey |
| LYS | 1 | Grey |
| GLU | 1 | Grey |
| GLU | 1 | Grey |
| P70 | 1 | Red |
| I71 | 1 | Green |
| H72 | 1 | Green |
| I75 | 1 | Green |
| T85 | 1 | Green |
| S86 | 1 | Green |
| K87 | 1 | Green |
| V101 | 1 | Green |
| L105 | 1 | Green |
| K109 | 1 | Green |
| F112 | 1 | Green |
| I113 | 1 | Green |
| I117 | 1 | Green |
| S118 | 1 | Green |
| N119 | 1 | Green |
| L131 | 1 | Green |
| A149 | 1 | Green |
| E150 | 1 | Green |
| K151 | 1 | Green |
| G152 | 1 | Green |
| T153 | 1 | Green |
| I161 | 1 | Green |
| G162 | 1 | Green |
| T174 | 1 | Green |
| R177 | 1 | Green |
| S180 | 1 | Green |
| K181 | 1 | Green |
| A182 | 1 | Green |
| F183 | 1 | Green |
| L184 | 1 | Green |
| D185 | 1 | Green |
| A186 | 1 | Green |
| LEU | 1 | Grey |
| GLN | 1 | Grey |
| ASN | 1 | Grey |
| GLN | 1 | Grey |
| A191 | 1 | Red |
| E192 | 1 | Red |
| A193 | 1 | Red |
| S194 | 1 | Red |
| I198 | 1 | Green |
| G199 | 1 | Green |
| S207 | 1 | Green |
| M210 | 1 | Green |
| V211 | 1 | Green |
| A212 | 1 | Green |
| D213 | 1 | Green |
| R214 | 1 | Green |
| V215 | 1 | Green |
| E216 | 1 | Green |
| R220 | 1 | Green |
| S221 | 1 | Green |
| A222 | 1 | Green |
| A223 | 1 | Green |
| S226 | 1 | Green |
| L227 | 1 | Green |
| G228 | 1 | Green |
| L232 | 1 | Green |
| E240 | 1 | Green |
| T241 | 1 | Green |
| A242 | 1 | Green |
| V247 | 1 | Green |
| R248 | 1 | Green |
| L255 | 1 | Green |
| H256 | 1 | Green |
| L257 | 1 | Green |
| R271 | 1 | Green |
| V274 | 1 | Green |
| T275 | 1 | Green |
| K276 | 1 | Green |
| V277 | 1 | Green |
| S278 | 1 | Green |
| N279 | 1 | Green |
| F280 | 1 | Green |
| V281 | 1 | Green |
| S282 | 1 | Green |
| F283 | 1 | Green |
| R290 | 1 | Green |
| R291 | 1 | Green |
| N292 | 1 | Green |
| N293 | 1 | Green |
| I298 | 1 | Green |
| V299 | 1 | Green |
| V300 | 1 | Green |
| K304 | 1 | Green |
| R307 | 1 | Green |
| E308 | 1 | Green |
| E312 | 1 | Green |
| R316 | 1 | Green |
| R326 | 1 | Green |
| Y327 | 1 | Green |
| K332 | 1 | Green |
| T333 | 1 | Green |
| D334 | 1 | Green |
| A335 | 1 | Green |
| P336 | 1 | Green |
| L337 | 1 | Green |
| N338 | 1 | Green |
| T339 | 1 | Green |
| L342 | 1 | Green |
| V345 | 1 | Green |
| P346 | 1 | Green |
| D347 | 1 | Green |
| K348 | 1 | Green |
| K349 | 1 | Green |
| P350 | 1 | Green |
| S351 | 1 | Green |
| M352 | 1 | Green |
| F353 | 1 | Green |
| ASP | 1 | Grey |
| VAL | 1 | Grey |
| SER | 1 | Grey |
| ARG | 1 | Grey |
| GLU | 1 | Grey |
| LEU | 1 | Grey |
| GLY | 1 | Grey |
| SER | 1 | Grey |
| S362 | 1 | Green |
| V363 | 1 | Green |
| S367 | 1 | Green |
| R368 | 1 | Green |
| K369 | 1 | Green |
| V370 | 1 | Green |
| K375 | 1 | Green |
| A376 | 1 | Green |
| T377 | 1 | Green |
| W383 | 1 | Green |
| L384 | 1 | Green |
| R388 | 1 | Green |
| G389 | 1 | Green |
| V390 | 1 | Green |
| E391 | 1 | Green |



• Molecule 1: Heat shock protein 75 kDa, mitochondrial



• Molecule 1: Heat shock protein 75 kDa, mitochondrial



D543	K544	K545	K546	L547	I548	S549	V550	GLU	THR	ASP	ILE	VAL	VAL	ASP	HIS	TYR	LYS	GLU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	115.55Å 115.55Å 339.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.82 – 3.30 37.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.82-3.30) 92.5 (37.82-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.220 , 0.285 0.229 , 0.289	Depositor DCC
R_{free} test set	1897 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14236	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: 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	0.51	1/2963 (0.0%)	1.27	28/3987 (0.7%)
1	B	0.48	0/3871	1.05	15/5213 (0.3%)
1	C	0.60	6/3859 (0.2%)	1.24	43/5198 (0.8%)
1	D	0.54	2/3677 (0.1%)	1.19	36/4948 (0.7%)
All	All	0.54	9/14370 (0.1%)	1.19	122/19346 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	4
1	D	0	1
All	All	0	12

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	550	VAL	CA-CB	8.77	1.65	1.54
1	C	497	ILE	CA-C	-7.53	1.43	1.52
1	C	498	TYR	CA-C	5.91	1.59	1.52
1	D	410	LEU	CA-C	5.85	1.60	1.52
1	D	498	TYR	CD1-CE1	-5.81	1.21	1.38
1	C	500	LEU	CA-C	-5.53	1.45	1.52
1	A	440	PHE	CA-C	-5.32	1.46	1.52
1	C	499	TYR	CA-C	5.20	1.60	1.53
1	C	499	TYR	CD1-CE1	5.06	1.53	1.38

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	LYS	CA-C-N	-18.71	96.45	119.84
1	A	349	LYS	C-N-CA	-18.71	96.45	119.84
1	C	498	TYR	N-CA-C	12.46	126.80	108.60
1	C	191	ALA	N-CA-C	11.76	143.91	111.00
1	D	308	GLU	CA-C-N	-11.35	107.58	122.79
1	D	308	GLU	C-N-CA	-11.35	107.58	122.79
1	A	345	VAL	CA-C-N	11.14	131.95	120.14
1	A	345	VAL	C-N-CA	11.14	131.95	120.14
1	C	192	GLU	N-CA-CB	-11.04	93.79	109.91
1	C	520	LYS	N-CA-C	-10.89	99.44	113.17
1	C	498	TYR	CA-C-N	10.31	140.50	122.67
1	C	498	TYR	C-N-CA	10.31	140.50	122.67
1	C	497	ILE	CB-CA-C	-10.08	98.76	110.96
1	D	396	ILE	CA-C-N	10.05	130.69	119.83
1	D	396	ILE	C-N-CA	10.05	130.69	119.83
1	C	518	LYS	CA-C-N	-10.05	106.92	122.60
1	C	518	LYS	C-N-CA	-10.05	106.92	122.60
1	C	531	PHE	N-CA-C	-10.02	100.59	112.92
1	B	489	ARG	N-CA-C	9.75	125.00	113.20
1	A	448	MET	CA-C-N	-9.75	106.45	122.54
1	A	448	MET	C-N-CA	-9.75	106.45	122.54
1	C	345	VAL	CA-C-N	9.60	129.54	119.85
1	C	345	VAL	C-N-CA	9.60	129.54	119.85
1	A	347	ASP	N-CA-C	9.44	122.97	112.97
1	A	223	ALA	CA-C-N	8.93	131.00	119.84
1	A	223	ALA	C-N-CA	8.93	131.00	119.84
1	C	335	ALA	C-N-CD	-8.77	101.31	120.60
1	C	548	ILE	N-CA-C	8.68	122.07	108.87
1	D	345	VAL	CA-C-N	8.38	128.33	120.03
1	D	345	VAL	C-N-CA	8.38	128.33	120.03
1	A	436	LYS	N-CA-C	8.31	128.50	110.80
1	C	522	THR	N-CA-C	-8.14	97.53	110.14
1	D	498	TYR	CA-C-N	8.10	135.85	122.73
1	D	498	TYR	C-N-CA	8.10	135.85	122.73
1	A	349	LYS	N-CA-C	-8.06	99.85	110.40
1	C	335	ALA	CA-C-N	8.01	146.22	127.00
1	C	335	ALA	C-N-CA	8.01	146.22	127.00
1	C	548	ILE	O-C-N	-7.98	113.58	122.83
1	D	545	LYS	N-CA-C	-7.96	96.59	109.96
1	C	497	ILE	N-CA-CB	7.79	119.88	111.00
1	D	309	TRP	CA-CB-CG	7.78	128.38	113.60
1	A	434	ALA	N-CA-C	7.42	119.01	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	GLU	CA-C-N	7.41	135.69	121.54
1	A	435	GLU	C-N-CA	7.41	135.69	121.54
1	A	433	ASP	CA-C-N	7.38	130.03	120.44
1	A	433	ASP	C-N-CA	7.38	130.03	120.44
1	C	499	TYR	O-C-N	-7.36	114.30	122.84
1	D	394	GLU	CA-C-N	7.30	130.29	120.65
1	D	394	GLU	C-N-CA	7.30	130.29	120.65
1	D	309	TRP	N-CA-C	7.29	119.47	109.11
1	D	302	ASP	CA-C-N	7.26	128.92	119.84
1	D	302	ASP	C-N-CA	7.26	128.92	119.84
1	A	374	THR	CA-C-N	-7.24	112.91	123.05
1	A	374	THR	C-N-CA	-7.24	112.91	123.05
1	B	439	LYS	CD-CE-NZ	7.17	134.85	111.90
1	B	414	LEU	CA-CB-CG	7.15	141.33	116.30
1	D	395	ASP	N-CA-C	7.08	118.68	110.97
1	C	498	TYR	N-CA-CB	-6.94	100.77	111.46
1	C	550	VAL	N-CA-C	-6.91	106.05	112.96
1	A	433	ASP	N-CA-C	6.91	119.67	108.76
1	B	345	VAL	CA-C-N	6.84	126.80	120.03
1	B	345	VAL	C-N-CA	6.84	126.80	120.03
1	B	411	ILE	CG1-CB-CG2	-6.84	90.18	110.70
1	C	551	GLU	N-CA-C	-6.69	105.19	113.15
1	D	407	GLU	N-CA-C	-6.64	100.63	110.46
1	C	500	LEU	N-CA-C	-6.63	98.58	108.99
1	A	441	PHE	CA-C-N	-6.56	112.37	122.60
1	A	441	PHE	C-N-CA	-6.56	112.37	122.60
1	D	75	ILE	N-CA-C	6.51	117.89	107.73
1	D	312	GLU	N-CA-CB	-6.51	100.58	110.01
1	D	310	GLN	N-CA-C	-6.34	104.74	113.18
1	D	499	TYR	CA-C-N	-6.33	112.74	122.62
1	D	499	TYR	C-N-CA	-6.33	112.74	122.62
1	C	379	ILE	N-CA-C	-6.24	107.78	113.71
1	D	499	TYR	O-C-N	-6.23	115.67	123.27
1	C	497	ILE	CA-C-N	-6.15	111.28	121.80
1	C	497	ILE	C-N-CA	-6.15	111.28	121.80
1	D	499	TYR	N-CA-C	6.13	119.48	109.24
1	C	548	ILE	CB-CA-C	-6.07	102.89	111.21
1	B	194	SER	N-CA-C	-6.06	105.84	113.18
1	B	352	MET	N-CA-C	-5.92	105.72	113.17
1	B	494	THR	N-CA-C	-5.89	101.74	110.46
1	C	548	ILE	CA-C-N	-5.88	108.98	121.32
1	C	548	ILE	C-N-CA	-5.88	108.98	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	312	GLU	CA-CB-CG	5.85	125.80	114.10
1	B	520	LYS	N-CA-C	-5.84	105.34	112.88
1	D	304	LYS	CB-CG-CD	5.84	124.73	111.30
1	C	410	LEU	N-CA-C	5.83	120.23	113.18
1	C	375	LYS	CA-C-N	-5.79	113.00	122.26
1	C	375	LYS	C-N-CA	-5.79	113.00	122.26
1	C	494	THR	CA-C-N	-5.63	112.77	122.79
1	C	494	THR	C-N-CA	-5.63	112.77	122.79
1	C	308	GLU	N-CA-C	5.59	122.71	110.80
1	A	153	THR	N-CA-C	5.59	117.68	109.24
1	D	195	SER	N-CA-C	-5.57	106.33	113.01
1	B	151	LYS	N-CA-C	-5.52	106.52	113.20
1	A	451	GLY	CA-C-N	-5.49	113.89	122.56
1	A	451	GLY	C-N-CA	-5.49	113.89	122.56
1	B	149	ALA	CA-C-N	-5.46	111.90	122.06
1	B	149	ALA	C-N-CA	-5.46	111.90	122.06
1	C	334	ASP	N-CA-C	-5.45	103.90	110.88
1	D	199	GLY	N-CA-C	5.45	119.52	112.54
1	B	519	LYS	CA-C-N	-5.41	114.16	122.60
1	B	519	LYS	C-N-CA	-5.41	114.16	122.60
1	C	499	TYR	N-CA-C	5.40	118.45	110.46
1	A	430	SER	CA-C-N	-5.38	113.70	122.26
1	A	430	SER	C-N-CA	-5.38	113.70	122.26
1	C	550	VAL	CB-CA-C	-5.31	106.38	111.06
1	C	191	ALA	CB-CA-C	-5.31	102.54	110.50
1	A	322	HIS	CB-CA-C	5.29	120.10	112.05
1	C	374	THR	N-CA-C	-5.24	105.65	111.36
1	D	312	GLU	N-CA-C	5.24	116.67	111.07
1	D	497	ILE	CA-C-N	-5.21	113.70	122.29
1	D	497	ILE	C-N-CA	-5.21	113.70	122.29
1	D	303	PRO	CA-C-N	5.20	127.97	120.38
1	D	303	PRO	C-N-CA	5.20	127.97	120.38
1	D	475	LEU	CA-C-N	5.17	125.45	119.92
1	D	475	LEU	C-N-CA	5.17	125.45	119.92
1	C	530	GLN	CA-C-N	-5.14	114.43	122.65
1	C	530	GLN	C-N-CA	-5.14	114.43	122.65
1	A	440	PHE	CA-C-O	-5.05	115.61	121.07
1	D	304	LYS	N-CA-C	5.02	118.18	111.75

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	GLU	Peptide
1	A	434	ALA	Peptide
1	A	449	ARG	Peptide
1	A	452	ILE	Peptide
1	B	411	ILE	Peptide
1	B	412	ARG	Peptide
1	B	413	LYS	Peptide
1	C	307	ARG	Peptide
1	C	497	ILE	Peptide
1	C	530	GLN	Peptide
1	C	548	ILE	Mainchain
1	D	407	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2911	0	2936	153	0
1	B	3798	0	3799	152	0
1	C	3787	0	3793	186	0
1	D	3612	0	3625	177	0
2	A	31	0	13	1	0
2	B	31	0	13	0	0
2	C	31	0	13	1	0
2	D	31	0	13	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	14236	0	14205	650	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 23.

All (650) 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:498:TYR:CZ	1:C:549:SER:HA	1.97	0.99
1:B:228:GLY:HA3	1:B:247:VAL:HG21	1.46	0.98
1:C:497:ILE:HG13	1:C:545:LYS:HD2	1.48	0.95
1:D:408:SER:O	1:D:410:LEU:N	1.99	0.94
1:B:411:ILE:HG22	1:B:415:ARG:NH1	1.82	0.94
1:B:411:ILE:HG22	1:B:415:ARG:HH11	1.28	0.94
1:C:337:LEU:HD11	1:C:395:ASP:HB2	1.51	0.93
1:D:410:LEU:HG	1:D:413:LYS:HE2	1.49	0.93
1:B:174:THR:HG22	1:D:91:GLN:HB2	1.55	0.89
1:D:304:LYS:HG2	1:D:305:ASP:N	1.88	0.88
1:C:498:TYR:CE1	1:C:549:SER:HA	2.08	0.87
1:C:518:LYS:O	1:C:521:ASP:HB2	1.74	0.87
1:C:439:LYS:HA	1:C:442:GLU:HG3	1.57	0.87
1:D:362:SER:OG	1:D:388:ARG:NH1	2.07	0.86
1:D:361:SER:OG	1:D:362:SER:N	2.08	0.86
1:B:290:ARG:HD3	1:B:291:ARG:N	1.90	0.86
1:C:498:TYR:O	1:C:524:VAL:HA	1.75	0.86
1:C:300:MET:SD	1:C:340:ARG:NH2	2.48	0.86
1:C:529:GLU:O	1:C:531:PHE:N	2.09	0.85
1:D:312:GLU:OE1	1:D:313:GLU:HG2	1.77	0.84
1:D:381:PRO:HA	1:D:415:ARG:HH22	1.42	0.84
1:B:393:SER:HB3	1:B:396:ILE:HG12	1.60	0.83
1:C:362:SER:HB2	1:C:388:ARG:HH12	1.42	0.83
1:D:498:TYR:CD1	1:D:499:TYR:N	2.46	0.83
1:D:336:PRO:O	1:D:337:LEU:HB3	1.78	0.83
1:B:220:ARG:HD2	1:B:247:VAL:HG23	1.61	0.83
1:C:499:TYR:CE1	1:C:536:LEU:HB3	2.14	0.83
1:A:327:TYR:OH	1:A:440:PHE:HE2	1.62	0.83
1:C:393:SER:HB3	1:C:396:ILE:HG12	1.60	0.82
1:D:334:ASP:HA	1:D:337:LEU:O	1.80	0.81
1:D:410:LEU:HA	1:D:413:LYS:HG2	1.63	0.81
1:D:313:GLU:OE2	1:D:316:ARG:NH2	2.13	0.81
1:C:316:ARG:NH1	1:C:323:ASP:O	2.14	0.80
1:C:498:TYR:CE2	1:C:499:TYR:O	2.34	0.80
1:B:312:GLU:HB3	1:B:316:ARG:HH12	1.46	0.80
1:B:413:LYS:HG3	1:B:415:ARG:H	1.46	0.80
1:C:540:ARG:NH2	1:C:541:GLU:OE2	2.16	0.79
1:C:498:TYR:CD2	1:C:550:VAL:HG13	2.17	0.79
1:D:131:LEU:HB3	1:D:138:LEU:HD11	1.64	0.79
1:A:85:THR:HG22	1:C:242:ALA:HB2	1.63	0.79
1:C:486:TYR:OH	1:C:523:GLU:O	1.98	0.79
1:A:154:ILE:HG22	1:A:255:ILE:HB	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:TYR:CD1	1:C:536:LEU:HD13	2.17	0.79
1:A:298:ILE:HA	1:A:301:MET:HE3	1.66	0.78
1:A:436:LYS:O	1:A:438:ALA:N	2.16	0.78
1:C:542:PHE:O	1:C:545:LYS:NZ	2.17	0.78
1:C:449:ARG:NH1	1:C:532:ASP:OD1	2.17	0.78
1:C:498:TYR:CE2	1:C:550:VAL:N	2.51	0.78
1:B:411:ILE:CG2	1:B:415:ARG:HH11	1.95	0.77
1:B:412:ARG:CZ	1:B:415:ARG:HH21	1.97	0.77
1:D:307:ARG:N	1:D:310:GLN:OE1	2.19	0.77
1:D:302:ASP:HB2	1:D:304:LYS:HD2	1.67	0.76
1:C:327:TYR:CE1	1:C:429:GLN:HG2	2.20	0.76
1:B:414:LEU:HA	1:B:417:VAL:HB	1.68	0.76
1:B:413:LYS:HD2	1:B:414:LEU:HB3	1.67	0.76
1:B:469:ARG:NH1	1:B:482:SER:OG	2.20	0.75
1:C:490:MET:C	1:C:491:ARG:HG3	2.12	0.75
1:A:434:ALA:O	1:A:436:LYS:HG3	1.86	0.74
1:C:515:GLU:HG3	1:C:518:LYS:NZ	2.03	0.74
1:A:381:PRO:HG2	1:A:384:LEU:HD12	1.66	0.74
1:A:271:ARG:NH2	1:A:290:ARG:HD3	2.02	0.74
1:A:412:ARG:O	1:A:415:ARG:HB3	1.87	0.73
1:C:498:TYR:CG	1:C:548:ILE:O	2.40	0.73
1:D:410:LEU:HA	1:D:413:LYS:CG	2.19	0.73
1:C:498:TYR:CE2	1:C:550:VAL:HG13	2.24	0.73
1:D:381:PRO:CA	1:D:415:ARG:HH22	2.01	0.73
1:D:184:LEU:HD22	1:D:194:SER:HB3	1.71	0.73
1:A:378:ASP:HB3	1:A:415:ARG:HH21	1.52	0.73
1:C:327:TYR:HE1	1:C:429:GLN:HG2	1.54	0.73
1:A:327:TYR:HH	1:A:440:PHE:HE2	0.79	0.72
1:A:326:ARG:HG2	1:A:347:ASP:OD1	1.88	0.72
1:D:530:GLN:HG2	1:D:531:PHE:HA	1.72	0.72
1:A:324:LYS:HG2	1:A:325:PRO:HD2	1.71	0.72
1:A:378:ASP:HB3	1:A:415:ARG:NH2	2.05	0.72
1:B:351:SER:OG	1:B:352:MET:N	2.20	0.71
1:C:499:TYR:CG	1:C:536:LEU:HD13	2.24	0.71
1:C:497:ILE:HG22	1:C:498:TYR:HA	1.71	0.71
1:D:362:SER:O	1:D:375:LYS:HE3	1.90	0.71
1:B:240:GLU:HB3	1:D:87:LYS:HD3	1.72	0.71
1:D:435:GLU:C	1:D:439:LYS:HZ2	1.98	0.71
1:C:471:GLU:OE2	1:C:505:ARG:NH1	2.23	0.71
1:D:498:TYR:CE1	1:D:499:TYR:O	2.44	0.71
1:D:312:GLU:HG2	1:D:324:LYS:HD2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ARG:NE	1:D:93:GLU:OE2	2.22	0.70
1:D:407:GLU:HB2	1:D:412:ARG:HH12	1.55	0.70
1:B:411:ILE:HA	1:B:413:LYS:HD3	1.73	0.70
1:B:413:LYS:HZ1	1:B:415:ARG:HG2	1.56	0.70
1:C:321:ALA:C	1:C:322:HIS:HD2	1.99	0.70
1:D:128:ARG:HA	1:D:138:LEU:HD22	1.72	0.70
1:C:498:TYR:CG	1:C:499:TYR:N	2.58	0.69
1:B:412:ARG:CZ	1:B:415:ARG:NH2	2.55	0.69
1:C:362:SER:HB2	1:C:388:ARG:NH1	2.07	0.69
1:A:435:GLU:HB3	1:A:440:PHE:CZ	2.26	0.69
1:B:450:GLU:HA	1:D:353:PHE:HZ	1.57	0.69
1:C:549:SER:HB3	1:C:552:THR:OG1	1.93	0.69
1:A:363:VAL:HG22	1:A:364:ALA:H	1.55	0.69
1:C:497:ILE:O	1:C:498:TYR:HB2	1.91	0.69
1:D:168:LEU:HD13	1:D:231:TRP:HB2	1.74	0.69
1:A:96:LYS:HA	1:A:99:ASP:OD1	1.93	0.69
1:A:326:ARG:CZ	1:A:347:ASP:HA	2.22	0.69
1:B:494:THR:HG22	1:B:495:ARG:H	1.57	0.69
1:C:481:THR:OG1	1:C:489:ARG:NH2	2.26	0.69
1:D:303:PRO:HB3	1:D:330:HIS:HB3	1.74	0.68
1:C:336:PRO:HD3	1:C:417:VAL:HG21	1.75	0.68
1:B:283:PHE:O	1:B:293:ASN:ND2	2.27	0.68
1:B:490:MET:SD	1:B:491:ARG:N	2.67	0.68
1:B:242:ALA:HB2	1:D:85:THR:HG22	1.76	0.68
1:C:515:GLU:HG3	1:C:518:LYS:HZ1	1.58	0.68
1:D:312:GLU:CD	1:D:316:ARG:HH12	2.01	0.67
1:D:199:GLY:HA3	2:D:801:ANP:HNB1	1.59	0.67
1:B:449:ARG:NE	1:B:532:ASP:OD1	2.26	0.67
1:A:349:LYS:HD3	1:A:349:LYS:N	2.09	0.67
1:C:326:ARG:NH2	1:C:443:ASP:OD1	2.28	0.66
1:D:362:SER:OG	1:D:375:LYS:HE3	1.95	0.66
1:A:315:TYR:OH	1:A:346:PRO:HB3	1.95	0.66
1:B:411:ILE:HG22	1:B:415:ARG:CZ	2.25	0.66
1:B:450:GLU:HA	1:D:353:PHE:CZ	2.31	0.66
1:B:469:ARG:CZ	1:B:482:SER:OG	2.43	0.66
1:D:212:ALA:HB2	1:D:255:ILE:HG23	1.78	0.66
1:D:335:ALA:O	1:D:336:PRO:C	2.38	0.66
1:D:337:LEU:CD1	1:D:339:ILE:HG13	2.25	0.66
1:D:298:ILE:HG23	1:D:306:VAL:HG11	1.78	0.66
1:D:490:MET:HB2	1:D:494:THR:OG1	1.95	0.66
1:A:441:PHE:HD2	1:A:444:TYR:HB2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:HH21	1:A:290:ARG:HD3	1.60	0.65
1:C:329:LEU:HD21	1:C:331:TYR:HB2	1.77	0.65
1:A:444:TYR:HA	1:A:447:PHE:HD2	1.62	0.65
1:A:433:ASP:OD1	1:A:434:ALA:N	2.29	0.65
1:D:333:THR:HG23	1:D:335:ALA:H	1.62	0.64
1:A:168:LEU:HD13	1:A:231:TRP:HB2	1.78	0.64
1:B:490:MET:HE3	1:B:491:ARG:HB3	1.80	0.64
1:C:375:LYS:HG2	1:C:375:LYS:O	1.98	0.64
1:A:407:GLU:H	1:A:407:GLU:CD	2.06	0.63
1:B:439:LYS:HG3	1:B:442:GLU:HB2	1.80	0.63
1:D:124:LEU:HD22	1:D:141:MET:HB3	1.79	0.63
1:A:176:ALA:O	1:C:96:LYS:HE3	1.97	0.63
1:A:348:MET:C	1:A:349:LYS:HD3	2.24	0.63
1:D:498:TYR:HE1	1:D:499:TYR:O	1.78	0.63
1:A:101:VAL:HG13	1:A:105:LEU:HD23	1.81	0.63
1:C:490:MET:C	1:C:491:ARG:CG	2.72	0.63
1:D:335:ALA:O	1:D:337:LEU:N	2.31	0.63
1:D:393:SER:OG	1:D:395:ASP:HB3	1.98	0.63
1:A:316:ARG:NH2	1:A:323:ASP:O	2.32	0.63
1:C:368:ARG:NH1	1:C:394:GLU:O	2.32	0.63
1:D:184:LEU:HD21	1:D:197:ILE:HB	1.81	0.63
1:C:298:ILE:HD12	1:C:314:PHE:HB2	1.81	0.62
1:D:381:PRO:HB3	1:D:415:ARG:HH12	1.64	0.62
1:D:498:TYR:CE1	1:D:549:SER:HA	2.34	0.62
1:D:145:LEU:HD13	1:D:285:LEU:HD21	1.81	0.62
1:A:330:HIS:HA	1:A:342:ILE:HG13	1.80	0.62
1:D:498:TYR:HB2	1:D:548:ILE:HB	1.81	0.61
1:D:312:GLU:OE2	1:D:316:ARG:NH2	2.31	0.61
1:A:124:LEU:HD22	1:A:141:MET:HB3	1.80	0.61
1:A:442:GLU:C	1:A:444:TYR:H	2.08	0.61
1:B:307:ARG:CG	1:B:308:GLU:H	2.13	0.61
1:B:526:PHE:HB3	1:B:528:PHE:CZ	2.36	0.61
1:C:498:TYR:CE2	1:C:549:SER:HA	2.35	0.61
1:D:530:GLN:CG	1:D:531:PHE:HA	2.30	0.61
1:C:378:ASP:HB2	1:C:415:ARG:HH21	1.65	0.60
1:B:290:ARG:HD3	1:B:290:ARG:C	2.27	0.60
1:C:232:LEU:HD12	1:C:240:GLU:HG3	1.83	0.60
1:D:409:ALA:O	1:D:413:LYS:HG2	2.01	0.60
1:A:435:GLU:HB3	1:A:440:PHE:CE2	2.36	0.60
1:C:501:CYS:SG	1:C:533:GLU:HB2	2.42	0.60
1:A:327:TYR:CE2	1:A:429:GLN:HG2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:SER:O	1:C:491:ARG:HD3	2.02	0.60
1:C:498:TYR:CE1	1:C:499:TYR:CG	2.89	0.60
1:B:411:ILE:HA	1:B:413:LYS:CD	2.32	0.60
1:B:199:GLY:HA2	1:B:402:ARG:HH22	1.66	0.59
1:C:177:ARG:HH21	1:C:179:GLY:HA2	1.67	0.59
1:C:486:TYR:CD2	1:C:497:ILE:HG12	2.37	0.59
1:D:148:ASN:OD1	1:D:151:LYS:HG3	2.02	0.59
1:A:223:ALA:O	1:A:226:SER:OG	2.19	0.59
1:C:490:MET:O	1:C:491:ARG:CG	2.50	0.59
1:C:504:ASN:OD1	1:C:505:ARG:N	2.35	0.59
1:D:498:TYR:HD1	1:D:548:ILE:O	1.85	0.59
1:A:438:ALA:O	1:A:442:GLU:HB2	2.02	0.59
1:B:469:ARG:NH1	1:B:482:SER:HG	1.99	0.59
1:C:498:TYR:HD2	1:C:550:VAL:HG13	1.65	0.59
1:D:497:ILE:O	1:D:547:LEU:HA	2.02	0.59
1:B:307:ARG:HG3	1:B:308:GLU:H	1.67	0.59
1:B:491:ARG:NH1	1:B:492:ALA:HB3	2.18	0.59
1:D:327:TYR:HB2	1:D:345:VAL:HB	1.85	0.59
1:B:338:ASN:HD22	1:B:393:SER:HA	1.67	0.59
1:B:413:LYS:HD2	1:B:414:LEU:HD23	1.84	0.59
1:C:498:TYR:HE1	1:C:499:TYR:CZ	2.21	0.59
1:A:349:LYS:HG3	1:A:443:ASP:CG	2.28	0.58
1:B:412:ARG:NH1	1:B:415:ARG:HH21	2.01	0.58
1:C:321:ALA:C	1:C:322:HIS:CD2	2.80	0.58
1:D:498:TYR:OH	1:D:550:VAL:HB	2.03	0.58
1:A:324:LYS:CG	1:A:325:PRO:HD2	2.33	0.58
1:C:498:TYR:CD1	1:C:548:ILE:O	2.56	0.58
1:C:517:MET:HE3	1:C:550:VAL:HG12	1.85	0.58
1:C:271:ARG:HG3	1:C:292:MET:HE1	1.84	0.58
1:C:498:TYR:CE1	1:C:499:TYR:CD1	2.92	0.58
1:C:326:ARG:N	1:C:345:VAL:O	2.36	0.58
1:C:445:GLY:O	1:C:449:ARG:HG3	2.04	0.58
1:D:337:LEU:HD11	1:D:339:ILE:HG13	1.85	0.58
1:A:153:THR:HG22	1:A:256:HIS:HA	1.86	0.58
1:D:439:LYS:H	1:D:439:LYS:HD2	1.69	0.58
1:A:330:HIS:CD2	1:A:342:ILE:HD11	2.39	0.57
1:B:413:LYS:CD	1:B:414:LEU:HB3	2.33	0.57
1:A:435:GLU:O	1:A:440:PHE:HB2	2.05	0.57
1:B:503:PRO:HG2	1:B:507:LEU:HD12	1.86	0.57
1:D:307:ARG:CG	1:D:310:GLN:HE22	2.17	0.57
1:D:309:TRP:HA	1:D:312:GLU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:PRO:HB3	1:D:415:ARG:NH1	2.19	0.57
1:A:382:LYS:HD3	1:A:382:LYS:N	2.19	0.57
1:D:337:LEU:HD11	1:D:339:ILE:CD1	2.35	0.57
1:D:498:TYR:CD1	1:D:548:ILE:O	2.57	0.57
1:B:410:LEU:O	1:B:413:LYS:HD3	2.05	0.57
1:C:506:HIS:O	1:C:510:HIS:HB2	2.05	0.57
1:A:299:TRP:HA	1:A:342:ILE:HD13	1.86	0.57
1:A:316:ARG:HH21	1:A:323:ASP:C	2.11	0.57
1:A:412:ARG:HB3	1:A:415:ARG:HD2	1.87	0.57
1:A:412:ARG:HD2	1:A:415:ARG:NH1	2.20	0.57
1:B:413:LYS:HG3	1:B:415:ARG:N	2.19	0.57
1:A:312:GLU:HB3	1:A:324:LYS:HE3	1.87	0.56
1:B:248:ARG:NH1	1:D:74:ILE:HD11	2.20	0.56
1:B:425:PHE:O	1:B:429:GLN:HG2	2.04	0.56
1:B:494:THR:CG2	1:B:495:ARG:H	2.18	0.56
1:B:496:ASN:CG	1:B:548:ILE:HD13	2.30	0.56
1:D:131:LEU:HD13	1:D:138:LEU:HG	1.87	0.56
1:A:435:GLU:HB3	1:A:440:PHE:CE1	2.41	0.56
1:B:411:ILE:HG23	1:B:413:LYS:HE3	1.87	0.56
1:A:245:SER:HB2	1:C:82:GLN:HE21	1.71	0.56
1:A:378:ASP:CB	1:A:415:ARG:HH21	2.17	0.56
1:D:302:ASP:OD1	1:D:332:LYS:NZ	2.29	0.56
1:B:312:GLU:HB3	1:B:316:ARG:NH1	2.20	0.56
1:D:184:LEU:HD22	1:D:194:SER:CB	2.35	0.56
1:C:497:ILE:HG13	1:C:545:LYS:CD	2.31	0.56
1:B:339:ILE:HG12	1:B:414:LEU:HD13	1.88	0.56
1:A:316:ARG:NE	1:A:323:ASP:O	2.38	0.56
1:C:184:LEU:HD11	1:C:197:ILE:HB	1.88	0.56
1:C:339:ILE:HD13	1:C:418:LEU:HD21	1.87	0.56
1:C:471:GLU:HG3	1:C:479:GLN:O	2.06	0.56
1:D:128:ARG:HB2	1:D:141:MET:HE1	1.88	0.56
1:D:411:ILE:HG13	1:D:412:ARG:HH11	1.70	0.56
1:B:75:ILE:HD12	1:D:146:GLN:HB2	1.88	0.55
1:D:301:MET:C	1:D:332:LYS:HZ1	2.14	0.55
1:C:514:TYR:CD1	1:C:524:VAL:HG11	2.40	0.55
1:B:408:SER:O	1:B:410:LEU:N	2.39	0.55
1:B:494:THR:HG22	1:B:495:ARG:N	2.21	0.55
1:C:392:ASP:OD1	1:C:393:SER:N	2.39	0.55
1:A:326:ARG:NE	1:A:346:PRO:O	2.40	0.55
1:C:102:ALA:O	1:C:210:MET:HG2	2.05	0.55
2:A:801:ANP:O2B	2:A:801:ANP:O3'	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:THR:HG22	1:D:256:HIS:HA	1.89	0.55
1:D:95:LYS:O	1:D:99:ASP:HB2	2.06	0.54
1:B:552:THR:O	1:B:553:ASP:HB2	2.07	0.54
1:D:335:ALA:HB1	1:D:336:PRO:HD2	1.88	0.54
1:C:490:MET:O	1:C:491:ARG:HG2	2.08	0.54
1:A:323:ASP:OD1	1:A:324:LYS:N	2.39	0.54
1:C:326:ARG:HG3	1:C:347:ASP:HA	1.88	0.54
1:D:302:ASP:HB2	1:D:304:LYS:CD	2.38	0.54
1:B:223:ALA:HB3	1:B:226:SER:HB3	1.90	0.54
1:B:299:TRP:O	1:B:332:LYS:NZ	2.40	0.54
1:C:409:ALA:O	1:C:413:LYS:HG3	2.08	0.54
1:D:530:GLN:HA	1:D:532:ASP:H	1.73	0.54
1:B:308:GLU:O	1:B:312:GLU:HG3	2.08	0.54
1:C:514:TYR:CE1	1:C:518:LYS:HB2	2.43	0.54
1:D:164:THR:HG23	1:D:167:GLU:H	1.72	0.54
1:D:337:LEU:HD11	1:D:339:ILE:HD11	1.90	0.54
1:C:498:TYR:CE1	1:C:499:TYR:CE1	2.96	0.54
1:B:414:LEU:HD12	1:B:418:LEU:HD21	1.90	0.53
1:B:491:ARG:CZ	1:B:493:GLY:H	2.20	0.53
1:D:337:LEU:HD12	1:D:339:ILE:HG13	1.89	0.53
1:B:491:ARG:HB3	1:B:494:THR:OG1	2.09	0.53
1:C:498:TYR:CE1	1:C:499:TYR:CD2	2.96	0.53
1:A:314:PHE:O	1:A:318:VAL:HG12	2.09	0.53
1:D:435:GLU:O	1:D:439:LYS:HD2	2.08	0.53
1:B:393:SER:HB3	1:B:396:ILE:CG1	2.36	0.53
1:A:192:GLU:O	1:A:194:SER:N	2.41	0.53
1:C:333:THR:HG22	1:C:339:ILE:HB	1.91	0.53
1:B:214:ARG:HG3	1:B:256:HIS:HB2	1.91	0.53
1:D:435:GLU:HG2	1:D:439:LYS:NZ	2.23	0.53
1:B:333:THR:HB	1:B:339:ILE:HB	1.91	0.53
1:B:491:ARG:HH11	1:B:492:ALA:HB3	1.74	0.53
1:C:153:THR:HG22	1:C:256:HIS:HA	1.90	0.52
1:C:498:TYR:HE2	1:C:550:VAL:N	2.04	0.52
1:A:441:PHE:O	1:A:441:PHE:CD2	2.62	0.52
1:C:378:ASP:HB2	1:C:415:ARG:NH2	2.24	0.52
1:C:435:GLU:OE1	1:C:435:GLU:N	2.42	0.52
1:A:242:ALA:HB2	1:C:85:THR:HG22	1.91	0.52
1:B:375:LYS:HG3	1:B:377:THR:HG23	1.90	0.52
1:C:472:SER:OG	1:C:523:GLU:OE2	2.22	0.52
1:D:362:SER:O	1:D:375:LYS:CE	2.57	0.52
1:A:430:SER:HB3	1:A:437:TYR:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:HIS:CE1	1:C:187:LEU:HD11	2.45	0.52
1:A:363:VAL:HG13	1:A:376:ALA:HB3	1.92	0.52
1:A:440:PHE:O	1:A:441:PHE:C	2.50	0.52
1:D:326:ARG:HG2	1:D:345:VAL:O	2.09	0.52
1:D:378:ASP:HB3	1:D:382:LYS:NZ	2.24	0.52
1:B:180:SER:O	1:B:183:PHE:HB3	2.10	0.52
1:C:471:GLU:HG2	1:C:472:SER:H	1.75	0.52
1:A:217:VAL:HG22	1:A:253:ILE:HG12	1.91	0.52
1:A:411:ILE:O	1:A:414:LEU:HB3	2.10	0.52
1:C:326:ARG:N	1:C:347:ASP:OD1	2.42	0.52
1:C:471:GLU:HG2	1:C:472:SER:N	2.25	0.52
1:C:498:TYR:CD1	1:C:499:TYR:CD1	2.98	0.52
1:D:128:ARG:HA	1:D:138:LEU:CD2	2.38	0.52
1:D:275:THR:O	1:D:279:ASN:HB2	2.09	0.52
1:A:407:GLU:OE1	1:C:107:SER:HB2	2.10	0.51
1:C:498:TYR:CZ	1:C:549:SER:CA	2.85	0.51
1:C:498:TYR:HE1	1:C:499:TYR:CE1	2.27	0.51
1:D:392:ASP:OD1	1:D:393:SER:N	2.43	0.51
1:B:384:LEU:HD13	1:B:422:LEU:HD13	1.92	0.51
1:B:449:ARG:HB3	1:B:535:THR:OG1	2.10	0.51
1:D:126:LYS:HE2	1:D:180:SER:HA	1.92	0.51
1:B:411:ILE:HG23	1:B:413:LYS:CE	2.41	0.51
1:C:486:TYR:HE1	1:C:523:GLU:HG3	1.73	0.51
1:C:198:ILE:HA	1:C:368:ARG:HD3	1.93	0.51
1:C:517:MET:O	1:C:521:ASP:HA	2.11	0.51
1:D:546:LYS:HG3	1:D:547:LEU:N	2.25	0.51
1:C:498:TYR:HE2	1:C:550:VAL:H	1.59	0.51
1:B:327:TYR:HB2	1:B:345:VAL:HB	1.93	0.51
1:C:491:ARG:O	1:C:492:ALA:HB3	2.10	0.51
1:D:322:HIS:O	1:D:322:HIS:ND1	2.44	0.51
1:A:407:GLU:CD	1:A:407:GLU:N	2.69	0.51
1:C:420:GLN:O	1:C:424:LYS:HG3	2.11	0.51
1:C:550:VAL:C	1:C:552:THR:H	2.18	0.51
1:D:96:LYS:O	1:D:100:ILE:HG13	2.11	0.51
1:B:439:LYS:HA	1:B:442:GLU:HB2	1.93	0.51
1:C:530:GLN:CD	1:C:530:GLN:O	2.54	0.51
1:D:469:ARG:HB3	1:D:480:LEU:HD13	1.92	0.51
1:A:392:ASP:OD1	1:A:393:SER:N	2.45	0.50
1:B:408:SER:O	1:B:411:ILE:N	2.24	0.50
1:B:413:LYS:NZ	1:B:415:ARG:HG2	2.26	0.50
1:C:486:TYR:CE2	1:C:497:ILE:HG12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:GLU:CD	1:D:316:ARG:NH1	2.67	0.50
1:A:368:ARG:NH1	1:A:394:GLU:HB3	2.26	0.50
1:B:411:ILE:HG22	1:B:415:ARG:NE	2.27	0.50
1:A:330:HIS:CE1	1:A:342:ILE:HD11	2.46	0.50
1:B:333:THR:HG23	1:B:335:ALA:H	1.76	0.50
1:C:217:VAL:HG22	1:C:253:ILE:HG12	1.92	0.50
1:D:312:GLU:OE1	1:D:313:GLU:N	2.45	0.50
1:A:441:PHE:O	1:A:441:PHE:CG	2.65	0.50
1:D:490:MET:CB	1:D:494:THR:OG1	2.60	0.50
1:D:411:ILE:HG13	1:D:412:ARG:HD3	1.93	0.50
1:A:327:TYR:CZ	1:A:429:GLN:HG2	2.47	0.49
1:B:85:THR:HG22	1:D:242:ALA:HB2	1.93	0.49
1:D:395:ASP:C	1:D:395:ASP:OD1	2.54	0.49
1:C:275:THR:O	1:C:279:ASN:HB2	2.12	0.49
1:A:149:ALA:HA	1:A:265:SER:HB2	1.93	0.49
1:A:310:GLN:C	1:A:312:GLU:H	2.20	0.49
1:B:362:SER:HB2	1:B:388:ARG:NH1	2.27	0.49
1:B:481:THR:OG1	1:B:489:ARG:NH2	2.43	0.49
1:D:337:LEU:HD11	1:D:339:ILE:CG1	2.41	0.49
1:D:471:GLU:O	1:D:526:PHE:N	2.38	0.49
1:D:131:LEU:CD2	1:D:136:GLN:NE2	2.75	0.49
1:A:393:SER:O	1:A:396:ILE:HG12	2.13	0.49
1:C:127:LEU:HD23	1:C:141:MET:HE3	1.93	0.49
1:D:312:GLU:CD	1:D:316:ARG:HH22	2.18	0.49
1:A:231:TRP:HD1	1:A:241:ILE:HD11	1.78	0.49
1:B:406:GLN:O	1:B:411:ILE:HD12	2.12	0.49
1:C:396:ILE:HG21	1:C:405:LEU:HD11	1.95	0.49
1:C:407:GLU:HG3	1:C:411:ILE:HB	1.95	0.49
1:C:474:ALA:O	1:C:475:LEU:HD23	2.12	0.49
1:D:326:ARG:HD2	1:D:346:PRO:O	2.12	0.49
1:D:381:PRO:HG2	1:D:384:LEU:HD12	1.94	0.49
1:D:466:LYS:HD2	1:D:466:LYS:O	2.11	0.49
1:B:367:SER:O	1:B:370:VAL:HG12	2.12	0.49
1:B:471:GLU:HG2	1:B:479:GLN:O	2.12	0.49
1:C:283:PHE:O	1:C:293:ASN:ND2	2.45	0.49
1:C:336:PRO:CD	1:C:417:VAL:HG21	2.42	0.49
1:C:486:TYR:HE1	1:C:523:GLU:HB3	1.77	0.49
1:C:134:ASP:HB3	1:C:136:GLN:HG2	1.94	0.49
1:C:548:ILE:O	1:C:548:ILE:HG22	2.12	0.49
1:C:427:ILE:O	1:C:430:SER:OG	2.22	0.48
1:A:176:ALA:O	1:C:96:LYS:CE	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ALA:HB2	1:A:255:ILE:HG23	1.95	0.48
1:A:313:GLU:HA	1:A:316:ARG:HG3	1.95	0.48
1:B:307:ARG:CG	1:B:308:GLU:N	2.74	0.48
1:B:326:ARG:HG3	1:B:327:TYR:CD2	2.49	0.48
1:B:490:MET:CG	1:B:491:ARG:H	2.27	0.48
1:B:491:ARG:HD2	1:B:492:ALA:N	2.29	0.48
1:C:498:TYR:CD2	1:C:548:ILE:O	2.66	0.48
1:D:396:ILE:HA	1:D:397:PRO:HD3	1.57	0.48
1:D:546:LYS:HG2	1:D:548:ILE:HD12	1.95	0.48
1:C:482:SER:OG	1:C:485:GLU:HG3	2.13	0.48
1:C:518:LYS:NZ	1:C:519:LYS:HG3	2.28	0.48
1:A:430:SER:HB2	1:A:436:LYS:HE3	1.94	0.48
1:C:316:ARG:HH12	1:C:323:ASP:C	2.20	0.48
2:C:801:ANP:O1G	2:C:801:ANP:O3A	2.31	0.48
1:A:384:LEU:HD13	1:A:422:LEU:HD13	1.95	0.48
1:D:217:VAL:HG22	1:D:253:ILE:HG12	1.96	0.48
1:D:335:ALA:C	1:D:337:LEU:N	2.71	0.48
1:D:476:PRO:HD2	1:D:479:GLN:HB2	1.95	0.48
1:A:214:ARG:HH21	1:A:256:HIS:CE1	2.32	0.48
1:B:72:HIS:O	1:D:289:GLY:HA2	2.14	0.48
1:B:351:SER:OG	1:B:353:PHE:N	2.37	0.48
1:C:261:CYS:C	1:C:263:GLU:N	2.71	0.48
1:C:307:ARG:HG3	1:C:308:GLU:H	1.79	0.48
1:A:312:GLU:O	1:A:316:ARG:HG2	2.14	0.48
1:B:414:LEU:CA	1:B:417:VAL:HB	2.42	0.48
1:C:382:LYS:CD	1:C:382:LYS:H	2.27	0.48
1:B:153:THR:HG22	1:B:256:HIS:HA	1.96	0.48
1:D:99:ASP:CG	1:D:103:ARG:HH12	2.21	0.48
1:A:276:LYS:HD3	1:A:277:TYR:CZ	2.49	0.47
1:A:412:ARG:C	1:A:415:ARG:HB3	2.38	0.47
1:B:298:ILE:HG22	1:B:342:ILE:HD11	1.96	0.47
1:D:307:ARG:HG2	1:D:310:GLN:HE22	1.78	0.47
1:A:383:TRP:HB2	1:A:447:PHE:O	2.13	0.47
1:A:434:ALA:C	1:A:436:LYS:HG3	2.39	0.47
1:B:486:TYR:CE1	1:B:497:ILE:HG23	2.48	0.47
1:D:131:LEU:HD22	1:D:136:GLN:HB2	1.96	0.47
1:D:381:PRO:HB2	1:D:383:TRP:CD1	2.49	0.47
1:D:293:ASN:OD1	1:D:293:ASN:N	2.45	0.47
1:A:310:GLN:HA	1:A:312:GLU:HG2	1.95	0.47
1:A:330:HIS:CG	1:A:342:ILE:HD11	2.49	0.47
1:D:309:TRP:HA	1:D:312:GLU:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:THR:HA	1:D:378:ASP:HA	1.50	0.47
1:D:498:TYR:O	1:D:524:VAL:HA	2.14	0.47
1:A:327:TYR:HB2	1:A:345:VAL:HB	1.96	0.47
1:A:441:PHE:CD2	1:A:444:TYR:HB2	2.46	0.47
1:D:199:GLY:HA2	1:D:402:ARG:HH22	1.79	0.47
1:D:435:GLU:O	1:D:438:ALA:HB3	2.14	0.47
1:A:154:ILE:HD13	1:A:264:PHE:O	2.15	0.47
1:A:442:GLU:C	1:A:444:TYR:N	2.66	0.47
1:C:486:TYR:HD2	1:C:497:ILE:HG12	1.80	0.47
1:D:326:ARG:HB3	1:D:347:ASP:OD1	2.15	0.47
1:A:347:ASP:O	1:A:348:MET:SD	2.72	0.47
1:B:536:LEU:HD22	1:B:547:LEU:HD22	1.97	0.47
1:C:96:LYS:O	1:C:100:ILE:HG13	2.14	0.47
1:D:466:LYS:HE2	1:D:482:SER:OG	2.15	0.47
1:B:521:ASP:OD1	1:B:521:ASP:O	2.33	0.47
1:C:399:ASN:HA	1:C:406:GLN:HG3	1.96	0.46
1:A:310:GLN:C	1:A:312:GLU:N	2.72	0.46
1:A:312:GLU:HB3	1:A:324:LYS:CE	2.45	0.46
1:A:363:VAL:HG22	1:A:364:ALA:N	2.26	0.46
1:A:276:LYS:HD3	1:A:277:TYR:CE2	2.50	0.46
1:D:205:PHE:HE1	1:D:253:ILE:HD13	1.81	0.46
1:D:499:TYR:CE2	1:D:548:ILE:O	2.69	0.46
1:A:420:GLN:O	1:A:424:LYS:HG3	2.16	0.46
1:B:362:SER:HA	1:B:375:LYS:NZ	2.30	0.46
1:C:375:LYS:O	1:C:375:LYS:CG	2.62	0.46
1:C:428:ASP:O	1:C:432:LYS:HG3	2.15	0.46
1:C:486:TYR:HE1	1:C:523:GLU:CG	2.29	0.46
1:B:101:VAL:HG13	1:B:105:LEU:HD23	1.97	0.46
1:D:333:THR:CG2	1:D:335:ALA:H	2.26	0.46
1:C:150:GLU:H	1:C:150:GLU:HG3	1.51	0.46
1:D:543:ASP:O	1:D:545:LYS:HD3	2.16	0.46
1:A:179:GLY:HA2	1:A:182:ALA:HB3	1.98	0.46
1:A:444:TYR:HD1	1:A:447:PHE:CE2	2.34	0.46
1:B:408:SER:O	1:B:409:ALA:C	2.59	0.46
1:C:530:GLN:C	1:C:532:ASP:H	2.20	0.46
1:A:284:PRO:HB3	1:A:291:ARG:NH1	2.31	0.46
1:A:377:THR:HA	1:A:378:ASP:HA	1.48	0.46
1:A:438:ALA:O	1:A:440:PHE:O	2.33	0.46
1:C:299:TRP:HE1	1:C:300:MET:HE3	1.80	0.46
1:C:498:TYR:CE1	1:C:499:TYR:CE2	3.04	0.46
1:D:407:GLU:HB2	1:D:412:ARG:NH1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ARG:NE	1:B:415:ARG:NH2	2.64	0.45
1:B:435:GLU:O	1:B:438:ALA:HB3	2.17	0.45
1:D:302:ASP:C	1:D:304:LYS:N	2.74	0.45
1:D:312:GLU:O	1:D:315:TYR:HB3	2.16	0.45
1:D:449:ARG:HD3	1:D:532:ASP:OD1	2.16	0.45
1:D:482:SER:HB3	1:D:485:GLU:HG3	1.98	0.45
1:A:176:ALA:O	1:C:96:LYS:NZ	2.48	0.45
1:A:341:SER:C	1:A:342:ILE:HD12	2.40	0.45
1:D:150:GLU:CD	1:D:150:GLU:H	2.25	0.45
1:D:532:ASP:OD1	1:D:532:ASP:N	2.45	0.45
1:C:498:TYR:CD2	1:C:499:TYR:N	2.84	0.45
1:A:116:LEU:HD11	1:A:255:ILE:HD11	1.98	0.45
1:B:299:TRP:CD2	1:B:390:VAL:HG11	2.50	0.45
1:B:412:ARG:NE	1:B:415:ARG:HH21	2.12	0.45
1:D:99:ASP:CG	1:D:103:ARG:HH22	2.24	0.45
1:D:375:LYS:HD2	1:D:375:LYS:HA	1.44	0.45
1:A:378:ASP:CG	1:A:415:ARG:HH21	2.24	0.45
1:A:447:PHE:C	1:A:450:GLU:HB3	2.41	0.45
1:D:131:LEU:HB2	1:D:138:LEU:HD21	1.97	0.45
1:D:199:GLY:HA3	2:D:801:ANP:N3B	2.31	0.45
1:D:361:SER:N	1:D:377:THR:HG22	2.32	0.45
1:D:498:TYR:HD1	1:D:499:TYR:H	1.54	0.45
1:A:139:PRO:O	1:A:141:MET:HG3	2.17	0.45
1:B:180:SER:O	1:B:184:LEU:HD13	2.16	0.45
1:B:326:ARG:HB3	1:B:347:ASP:OD1	2.17	0.45
1:B:362:SER:HA	1:B:375:LYS:HZ2	1.82	0.45
1:C:383:TRP:CE2	1:C:384:LEU:HG	2.52	0.45
1:D:164:THR:OG1	1:D:165:GLN:N	2.50	0.45
1:D:472:SER:HA	1:D:525:LEU:HA	1.97	0.45
1:B:418:LEU:O	1:B:422:LEU:N	2.43	0.45
1:B:485:GLU:O	1:B:488:SER:HB3	2.17	0.45
1:A:164:THR:H	1:A:167:GLU:HB2	1.82	0.45
1:A:219:SER:HB2	1:A:251:THR:HG23	1.99	0.45
1:C:409:ALA:O	1:C:412:ARG:HG3	2.17	0.45
1:D:108:GLU:O	1:D:111:VAL:HG22	2.17	0.45
1:A:341:SER:O	1:A:342:ILE:HD12	2.17	0.44
1:C:261:CYS:C	1:C:263:GLU:H	2.24	0.44
1:D:399:ASN:HB3	1:D:404:LEU:HB3	2.00	0.44
1:D:498:TYR:CD1	1:D:498:TYR:C	2.94	0.44
1:C:168:LEU:HD13	1:C:231:TRP:HB2	1.99	0.44
1:A:284:PRO:HB3	1:A:291:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ILE:HG22	1:A:452:ILE:O	2.16	0.44
1:B:338:ASN:HD22	1:B:394:GLU:H	1.66	0.44
1:B:411:ILE:HD13	1:B:411:ILE:HG21	1.60	0.44
1:D:211:VAL:C	1:D:258:LYS:HG3	2.42	0.44
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.77	0.44
1:A:362:SER:O	1:A:388:ARG:HD2	2.17	0.44
1:B:198:ILE:HA	1:B:368:ARG:HD3	2.00	0.44
1:B:293:ASN:OD1	1:B:293:ASN:N	2.49	0.44
1:C:539:LEU:O	1:C:541:GLU:N	2.41	0.44
1:D:199:GLY:HA2	1:D:402:ARG:NH2	2.33	0.44
1:A:345:VAL:HA	1:A:346:PRO:HD3	1.57	0.44
1:B:383:TRP:HB2	1:B:447:PHE:O	2.17	0.44
1:A:184:LEU:HD21	1:A:197:ILE:HB	1.99	0.44
1:A:406:GLN:O	1:A:408:SER:N	2.51	0.44
1:B:207:SER:HB2	1:B:210:MET:HE2	1.98	0.44
1:B:349:LYS:HB2	1:B:349:LYS:HE2	1.69	0.44
1:C:394:GLU:H	1:C:394:GLU:HG3	1.54	0.44
1:D:498:TYR:O	1:D:524:VAL:HG23	2.17	0.44
1:A:104:SER:HA	1:C:406:GLN:NE2	2.33	0.44
1:A:338:ASN:OD1	1:A:338:ASN:C	2.61	0.44
1:B:161:ILE:HG22	1:B:162:GLY:O	2.18	0.44
1:B:276:LYS:HD3	1:B:277:TYR:CE2	2.53	0.44
1:D:499:TYR:HA	1:D:525:LEU:O	2.18	0.44
1:B:326:ARG:N	1:B:345:VAL:O	2.50	0.44
1:B:345:VAL:HA	1:B:346:PRO:HD3	1.74	0.44
1:C:181:LYS:HA	1:C:184:LEU:HB2	2.00	0.44
1:C:372:ILE:HG22	1:C:373:GLN:HG3	1.99	0.44
1:D:165:GLN:HB2	1:D:229:TYR:CE1	2.53	0.44
1:D:312:GLU:CG	1:D:324:LYS:HD2	2.43	0.44
1:B:299:TRP:HE1	1:B:300:MET:HE2	1.83	0.43
1:C:540:ARG:CZ	1:C:541:GLU:OE2	2.65	0.43
1:A:116:LEU:HB3	1:A:156:ILE:HD13	1.99	0.43
1:B:337:LEU:HD12	1:B:395:ASP:HB2	1.99	0.43
1:B:392:ASP:OD1	1:B:393:SER:N	2.51	0.43
1:C:518:LYS:C	1:C:521:ASP:HB2	2.40	0.43
1:D:355:VAL:HG11	1:D:446:LEU:HD13	1.99	0.43
1:A:365:LEU:HD13	1:A:405:LEU:HD11	1.99	0.43
1:B:412:ARG:HH11	1:B:415:ARG:HD2	1.83	0.43
1:B:491:ARG:NE	1:B:493:GLY:H	2.16	0.43
1:D:411:ILE:HG13	1:D:412:ARG:NH1	2.31	0.43
1:B:448:MET:H	1:B:448:MET:HG2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD22	1:C:141:MET:HB3	2.00	0.43
1:A:347:ASP:OD1	1:A:347:ASP:N	2.50	0.43
1:A:406:GLN:C	1:A:408:SER:H	2.26	0.43
1:A:442:GLU:OE2	1:A:442:GLU:O	2.37	0.43
1:C:486:TYR:CE1	1:C:490:MET:HE3	2.54	0.43
1:D:425:PHE:O	1:D:429:GLN:HG2	2.18	0.43
1:A:267:GLU:OE2	1:A:290:ARG:HD2	2.18	0.43
1:A:450:GLU:O	1:A:453:VAL:HB	2.17	0.43
1:C:212:ALA:HB2	1:C:255:ILE:HG23	2.00	0.43
1:C:349:LYS:N	1:C:349:LYS:HD3	2.33	0.43
1:C:393:SER:HB3	1:C:396:ILE:CG1	2.41	0.43
1:C:423:ILE:O	1:C:427:ILE:HG23	2.19	0.43
1:D:302:ASP:C	1:D:304:LYS:H	2.26	0.43
1:D:314:PHE:O	1:D:318:VAL:HG23	2.19	0.43
1:C:321:ALA:O	1:C:322:HIS:HD2	1.99	0.43
1:D:211:VAL:O	1:D:257:LEU:HA	2.19	0.43
1:D:466:LYS:HE2	1:D:484:SER:HB3	2.01	0.43
1:A:348:MET:HA	1:A:349:LYS:HD3	2.01	0.43
1:B:498:TYR:HB3	1:B:550:VAL:HG23	2.00	0.43
1:C:499:TYR:CE1	1:C:536:LEU:CB	2.94	0.43
1:D:334:ASP:CA	1:D:337:LEU:O	2.60	0.43
1:A:412:ARG:HD2	1:A:415:ARG:HH12	1.83	0.43
1:A:434:ALA:N	1:A:435:GLU:HG2	2.33	0.43
1:D:207:SER:HB2	1:D:210:MET:HE2	2.01	0.43
1:B:212:ALA:HB2	1:B:255:ILE:HG23	1.99	0.43
1:C:473:SER:OG	1:C:523:GLU:OE1	2.31	0.43
1:C:500:LEU:HD12	1:C:550:VAL:CG2	2.49	0.43
1:A:412:ARG:HB3	1:A:415:ARG:NH1	2.34	0.42
1:A:444:TYR:HD1	1:A:447:PHE:CD2	2.37	0.42
1:B:410:LEU:C	1:B:413:LYS:HB3	2.44	0.42
1:A:349:LYS:HB3	1:A:443:ASP:HB3	2.01	0.42
1:B:312:GLU:O	1:B:316:ARG:HG2	2.20	0.42
1:C:500:LEU:C	1:C:500:LEU:HD23	2.44	0.42
1:C:542:PHE:O	1:C:545:LYS:CE	2.66	0.42
1:A:315:TYR:CD2	1:A:325:PRO:HD3	2.54	0.42
1:A:412:ARG:HA	1:A:415:ARG:CB	2.49	0.42
1:B:211:VAL:O	1:B:257:LEU:HA	2.20	0.42
1:B:508:ALA:HB1	1:B:526:PHE:CD1	2.54	0.42
1:C:463:ASP:O	1:C:466:LYS:HG3	2.20	0.42
1:C:486:TYR:CE1	1:C:523:GLU:HB3	2.54	0.42
1:C:486:TYR:CE1	1:C:523:GLU:HG3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:O	1:A:197:ILE:HG12	2.18	0.42
1:A:214:ARG:NH2	1:A:256:HIS:ND1	2.67	0.42
1:A:286:TYR:HA	1:A:290:ARG:O	2.20	0.42
1:B:117:ILE:HD11	1:B:274:VAL:HG22	2.01	0.42
1:B:304:LYS:HB3	1:B:304:LYS:HE2	1.76	0.42
1:C:429:GLN:O	1:C:429:GLN:HG3	2.19	0.42
1:A:362:SER:OG	1:A:363:VAL:N	2.52	0.42
1:D:387:ILE:HD12	1:D:422:LEU:HD13	2.02	0.42
1:D:468:LEU:HD13	1:D:470:TYR:OH	2.19	0.42
1:C:498:TYR:HE2	1:C:550:VAL:HG13	1.79	0.42
1:D:460:VAL:O	1:D:464:ILE:HG13	2.19	0.42
1:A:433:ASP:C	1:A:435:GLU:HG2	2.45	0.42
1:B:517:MET:HG3	1:B:550:VAL:HG22	2.01	0.42
1:C:399:ASN:CA	1:C:406:GLN:HG3	2.50	0.42
1:D:319:ALA:HB1	1:D:388:ARG:HD2	2.02	0.42
1:A:164:THR:OG1	1:A:167:GLU:HG3	2.20	0.42
1:B:526:PHE:HB3	1:B:528:PHE:CE1	2.53	0.42
1:D:99:ASP:OD2	1:D:103:ARG:NH2	2.51	0.42
1:D:345:VAL:HA	1:D:346:PRO:HD3	1.69	0.42
1:A:436:LYS:C	1:A:438:ALA:H	2.18	0.42
1:C:316:ARG:HH12	1:C:323:ASP:CA	2.33	0.42
1:C:497:ILE:HG22	1:C:498:TYR:CA	2.46	0.42
1:A:205:PHE:HE1	1:A:253:ILE:HD13	1.85	0.41
1:B:221:SER:O	1:B:226:SER:OG	2.24	0.41
1:D:99:ASP:OD1	1:D:103:ARG:NH2	2.54	0.41
1:D:471:GLU:CD	1:D:528:PHE:HE2	2.28	0.41
1:B:275:THR:O	1:B:279:ASN:HB2	2.20	0.41
1:B:496:ASN:HB2	1:B:498:TYR:CZ	2.54	0.41
1:C:505:ARG:HA	1:C:528:PHE:CE1	2.55	0.41
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.84	0.41
1:D:362:SER:OG	1:D:388:ARG:CZ	2.65	0.41
1:A:138:LEU:HA	1:A:139:PRO:HD3	1.88	0.41
1:A:199:GLY:HA2	1:A:402:ARG:NH2	2.35	0.41
1:B:411:ILE:HA	1:B:413:LYS:CG	2.49	0.41
1:B:504:ASN:OD1	1:B:507:LEU:HG	2.21	0.41
1:C:348:MET:HE2	1:C:348:MET:HB3	1.78	0.41
1:D:500:LEU:HD23	1:D:524:VAL:HG21	2.02	0.41
1:A:365:LEU:CD1	1:A:405:LEU:HD11	2.50	0.41
1:B:271:ARG:HG3	1:B:292:MET:HE1	2.03	0.41
1:B:363:VAL:HG23	1:B:389:GLY:C	2.45	0.41
1:B:411:ILE:HG22	1:B:415:ARG:HE	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:LEU:HA	1:C:422:LEU:HD23	1.84	0.41
1:C:211:VAL:C	1:C:258:LYS:HG3	2.46	0.41
1:C:308:GLU:OE1	1:C:324:LYS:HE2	2.21	0.41
1:C:427:ILE:O	1:C:431:LYS:HG3	2.21	0.41
1:B:411:ILE:O	1:B:415:ARG:NH1	2.54	0.41
1:C:312:GLU:O	1:C:316:ARG:HB2	2.20	0.41
1:D:375:LYS:CE	1:D:388:ARG:HH12	2.34	0.41
1:B:413:LYS:CG	1:B:414:LEU:HB3	2.51	0.41
1:C:205:PHE:HE1	1:C:253:ILE:HD13	1.86	0.41
1:A:380:LEU:HA	1:A:381:PRO:HD2	1.76	0.41
1:C:298:ILE:HG22	1:C:342:ILE:HD11	2.03	0.41
1:D:445:GLY:HA2	1:D:448:MET:HE3	2.01	0.41
1:A:154:ILE:CD1	1:A:264:PHE:O	2.68	0.41
1:A:289:GLY:HA2	1:C:72:HIS:O	2.21	0.41
1:C:514:TYR:HD1	1:C:524:VAL:HG11	1.85	0.41
1:D:309:TRP:CA	1:D:312:GLU:HB3	2.50	0.41
2:D:801:ANP:C5'	2:D:801:ANP:O1B	2.59	0.41
1:A:180:SER:O	1:A:183:PHE:HB3	2.20	0.41
1:B:411:ILE:O	1:B:415:ARG:CZ	2.68	0.41
1:C:470:TYR:CD1	1:C:527:CYS:HB3	2.56	0.41
1:B:216:GLU:HG2	1:B:232:LEU:HD21	2.02	0.40
1:C:300:MET:CE	1:C:340:ARG:HH21	2.34	0.40
1:B:181:LYS:O	1:B:181:LYS:HG3	2.22	0.40
1:B:281:VAL:HG12	1:B:283:PHE:H	1.86	0.40
1:C:286:TYR:HA	1:C:290:ARG:O	2.21	0.40
1:C:497:ILE:HG21	1:C:497:ILE:HD13	1.70	0.40
1:A:406:GLN:C	1:A:408:SER:N	2.78	0.40
1:B:112:PHE:CG	1:B:113:ILE:N	2.89	0.40
1:A:88:HIS:O	1:C:238:VAL:HG13	2.22	0.40
1:A:91:GLN:HA	1:C:94:THR:HG21	2.03	0.40
1:B:412:ARG:HD3	1:B:412:ARG:HA	1.93	0.40
1:B:486:TYR:CD1	1:B:497:ILE:HG23	2.56	0.40
1:C:323:ASP:N	1:C:323:ASP:OD1	2.54	0.40
1:C:498:TYR:CE1	1:C:499:TYR:CZ	3.07	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	357/502 (71%)	310 (87%)	35 (10%)	12 (3%)	3	18
1	B	466/502 (93%)	433 (93%)	30 (6%)	3 (1%)	21	52
1	C	465/502 (93%)	442 (95%)	19 (4%)	4 (1%)	14	43
1	D	437/502 (87%)	412 (94%)	21 (5%)	4 (1%)	14	43
All	All	1725/2008 (86%)	1597 (93%)	105 (6%)	23 (1%)	9	35

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	PRO
1	A	293	ASN
1	A	336	PRO
1	A	435	GLU
1	A	437	TYR
1	B	414	LEU
1	C	530	GLN
1	D	336	PRO
1	D	409	ALA
1	C	521	ASP
1	D	337	LEU
1	A	350	PRO
1	A	436	LYS
1	B	413	LYS
1	C	492	ALA
1	B	521	ASP
1	A	294	THR
1	A	320	GLN
1	C	336	PRO
1	D	362	SER
1	A	441	PHE
1	A	83	GLY
1	A	363	VAL

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	318/443 (72%)	297 (93%)	21 (7%)	15	43
1	B	415/443 (94%)	396 (95%)	19 (5%)	24	53
1	C	414/443 (94%)	394 (95%)	20 (5%)	23	52
1	D	398/443 (90%)	380 (96%)	18 (4%)	24	53
All	All	1545/1772 (87%)	1467 (95%)	78 (5%)	22	50

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	103	ARG
1	A	128	ARG
1	A	131	LEU
1	A	150	GLU
1	A	154	ILE
1	A	196	LYS
1	A	214	ARG
1	A	240	GLU
1	A	256	HIS
1	A	282	SER
1	A	295	LEU
1	A	298	ILE
1	A	316	ARG
1	A	326	ARG
1	A	349	LYS
1	A	379	ILE
1	A	394	GLU
1	A	395	ASP
1	A	427	ILE
1	A	431	LYS
1	B	87	LYS
1	B	109	LYS
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	240	GLU
1	B	304	LYS
1	B	333	THR
1	B	334	ASP
1	B	394	GLU
1	B	405	LEU
1	B	408	SER
1	B	412	ARG
1	B	439	LYS
1	B	490	MET
1	B	495	ARG
1	B	520	LYS
1	B	527	CYS
1	B	548	ILE
1	B	550	VAL
1	B	552	THR
1	C	82	GLN
1	C	103	ARG
1	C	130	LYS
1	C	131	LEU
1	C	150	GLU
1	C	187	LEU
1	C	240	GLU
1	C	329	LEU
1	C	349	LYS
1	C	375	LYS
1	C	394	GLU
1	C	420	GLN
1	C	442	GLU
1	C	453	VAL
1	C	495	ARG
1	C	524	VAL
1	C	541	GLU
1	C	545	LYS
1	C	546	LYS
1	C	548	ILE
1	D	161	ILE
1	D	295	LEU
1	D	304	LYS
1	D	313	GLU
1	D	333	THR
1	D	337	LEU

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Mol	Chain	Res	Type
1	D	363	VAL
1	D	394	GLU
1	D	395	ASP
1	D	408	SER
1	D	411	ILE
1	D	412	ARG
1	D	431	LYS
1	D	466	LYS
1	D	479	GLN
1	D	480	LEU
1	D	524	VAL
1	D	548	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	HIS
1	B	322	HIS
1	C	129	HIS
1	C	322	HIS
1	C	338	ASN
1	C	479	GLN
1	C	538	HIS
1	D	136	GLN
1	D	256	HIS
1	D	279	ASN
1	D	330	HIS
1	D	538	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	ANP	B	801	3	33,33,33	1.04	5 (15%)	45,52,52	0.77	1 (2%)
2	ANP	A	801	3	33,33,33	2.05	6 (18%)	45,52,52	0.60	0
2	ANP	C	801	3	33,33,33	1.07	4 (12%)	45,52,52	0.53	1 (2%)
2	ANP	D	801	3	33,33,33	1.96	4 (12%)	45,52,52	2.11	6 (13%)

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
2	ANP	B	801	3	-	2/18/38/38	0/3/3/3
2	ANP	A	801	3	-	6/18/38/38	0/3/3/3
2	ANP	C	801	3	-	9/18/38/38	0/3/3/3
2	ANP	D	801	3	-	9/18/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	PG-O1G	7.93	1.58	1.46
2	D	801	ANP	PG-O1G	7.87	1.58	1.46
2	A	801	ANP	PB-O1B	6.66	1.56	1.46
2	D	801	ANP	PB-O1B	5.82	1.55	1.46
2	C	801	ANP	PB-O3A	-3.26	1.55	1.59
2	D	801	ANP	PB-O2B	-2.95	1.49	1.56
2	A	801	ANP	PB-O2B	-2.70	1.49	1.56
2	A	801	ANP	PG-O2G	-2.58	1.50	1.56
2	C	801	ANP	PG-O1G	2.55	1.50	1.46
2	B	801	ANP	PG-O1G	2.55	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	PG-N3B	2.53	1.70	1.63
2	B	801	ANP	PG-N3B	2.49	1.69	1.63
2	C	801	ANP	PG-N3B	2.47	1.69	1.63
2	B	801	ANP	PB-O3A	-2.45	1.56	1.59
2	D	801	ANP	PG-O2G	-2.40	1.50	1.56
2	C	801	ANP	PB-O1B	2.36	1.49	1.46
2	B	801	ANP	PB-O1B	2.22	1.49	1.46
2	A	801	ANP	PB-O3A	-2.21	1.56	1.59
2	B	801	ANP	PA-O3A	-2.03	1.57	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ANP	O1G-PG-N3B	-12.01	94.08	111.77
2	D	801	ANP	O1B-PB-N3B	-4.66	104.91	111.77
2	B	801	ANP	O1B-PB-N3B	-3.58	106.50	111.77
2	D	801	ANP	O5'-C5'-C4'	3.07	119.45	108.99
2	D	801	ANP	PA-O5'-C5'	-2.48	107.13	121.35
2	C	801	ANP	O3G-PG-O1G	-2.39	107.45	113.45
2	D	801	ANP	O3A-PA-O1A	2.28	117.57	110.70
2	D	801	ANP	O2B-PB-O3A	2.02	111.38	104.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	A	801	ANP	PG-N3B-PB-O1B
2	A	801	ANP	PA-O3A-PB-O2B
2	B	801	ANP	PB-N3B-PG-O1G
2	B	801	ANP	PA-O3A-PB-O2B
2	C	801	ANP	PB-N3B-PG-O1G
2	C	801	ANP	C5'-O5'-PA-O1A
2	C	801	ANP	C5'-O5'-PA-O3A
2	D	801	ANP	PB-N3B-PG-O1G
2	D	801	ANP	PA-O3A-PB-O1B
2	D	801	ANP	PA-O3A-PB-O2B
2	D	801	ANP	C5'-O5'-PA-O2A
2	A	801	ANP	O4'-C4'-C5'-O5'
2	A	801	ANP	C3'-C4'-C5'-O5'
2	C	801	ANP	PB-O3A-PA-O1A
2	D	801	ANP	O4'-C4'-C5'-O5'

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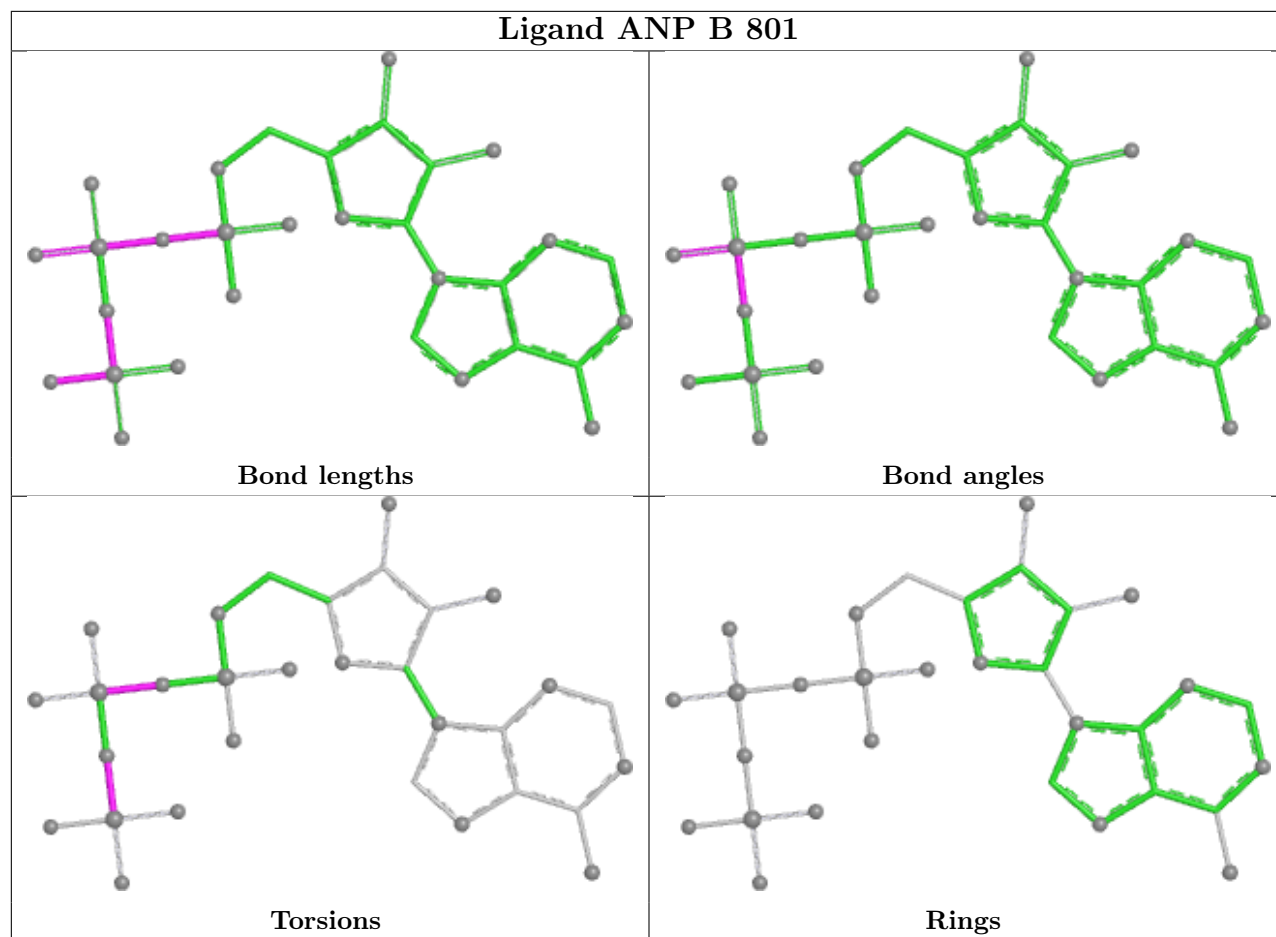
Mol	Chain	Res	Type	Atoms
2	C	801	ANP	PB-O3A-PA-O5'
2	D	801	ANP	PB-O3A-PA-O5'
2	D	801	ANP	C3'-C4'-C5'-O5'
2	C	801	ANP	C5'-O5'-PA-O2A
2	D	801	ANP	C5'-O5'-PA-O1A
2	C	801	ANP	PG-N3B-PB-O1B
2	D	801	ANP	PG-N3B-PB-O1B
2	C	801	ANP	C3'-C4'-C5'-O5'
2	A	801	ANP	PA-O3A-PB-O1B
2	C	801	ANP	O4'-C4'-C5'-O5'

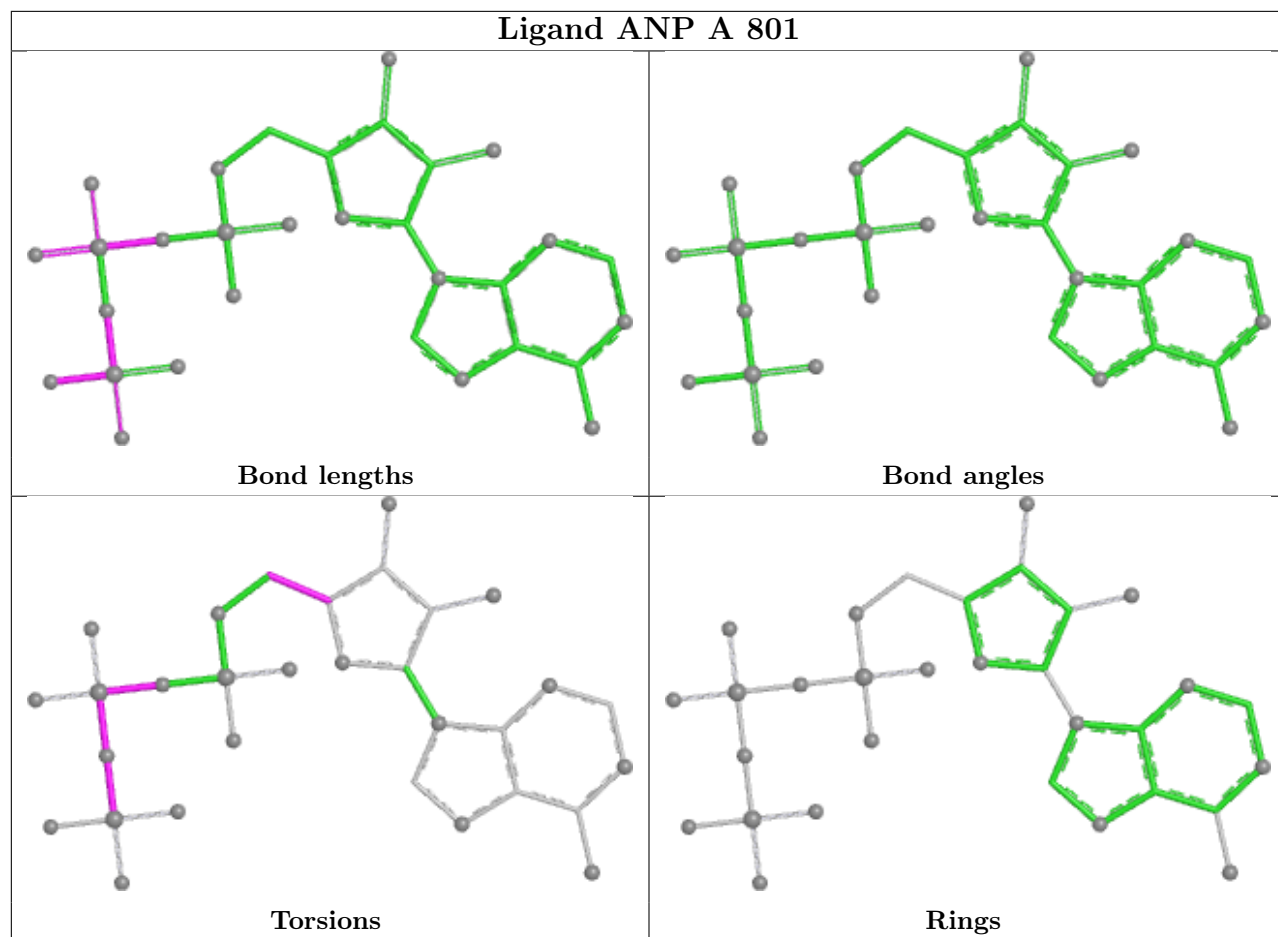
There are no ring outliers.

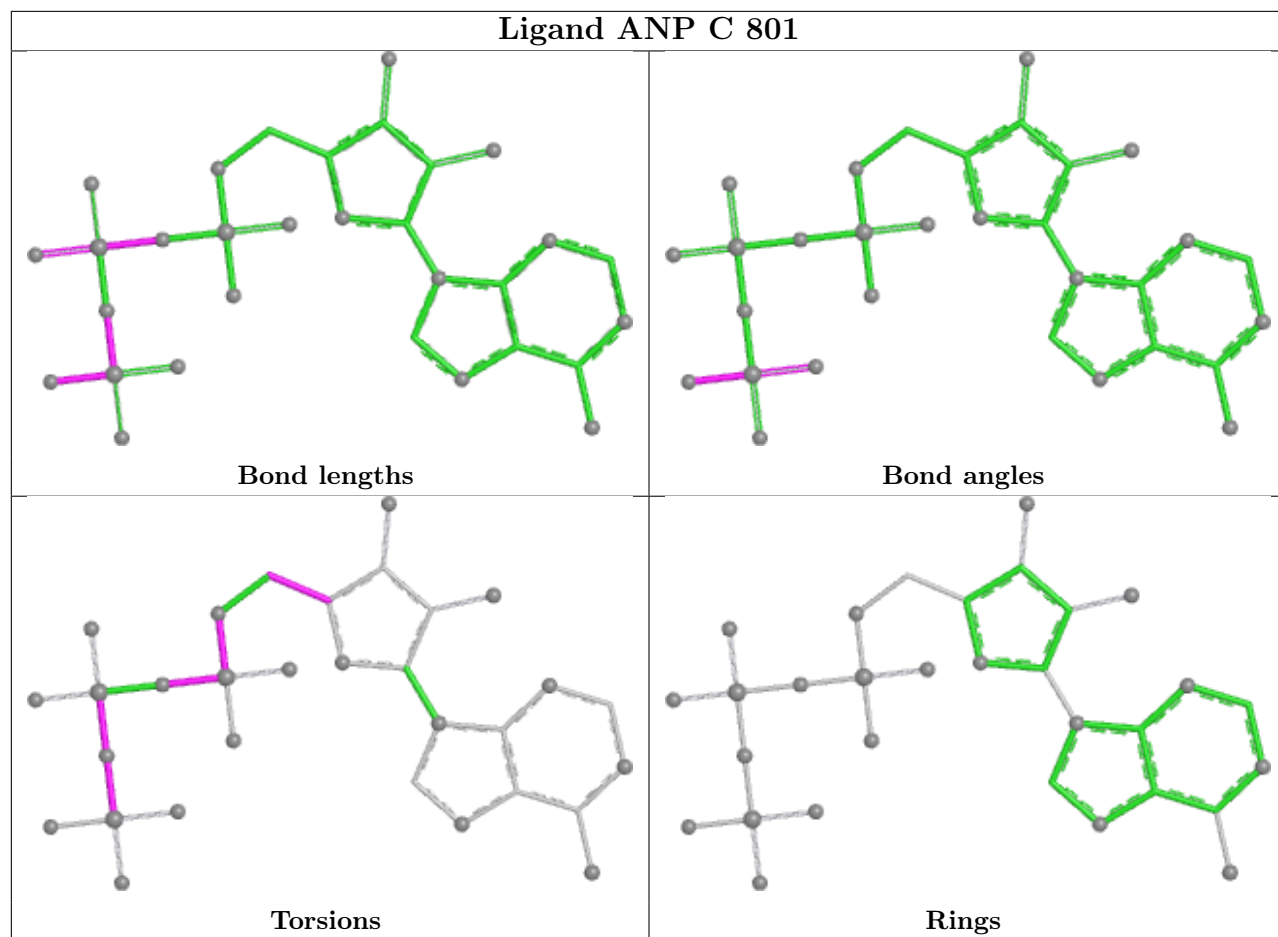
3 monomers are involved in 5 short contacts:

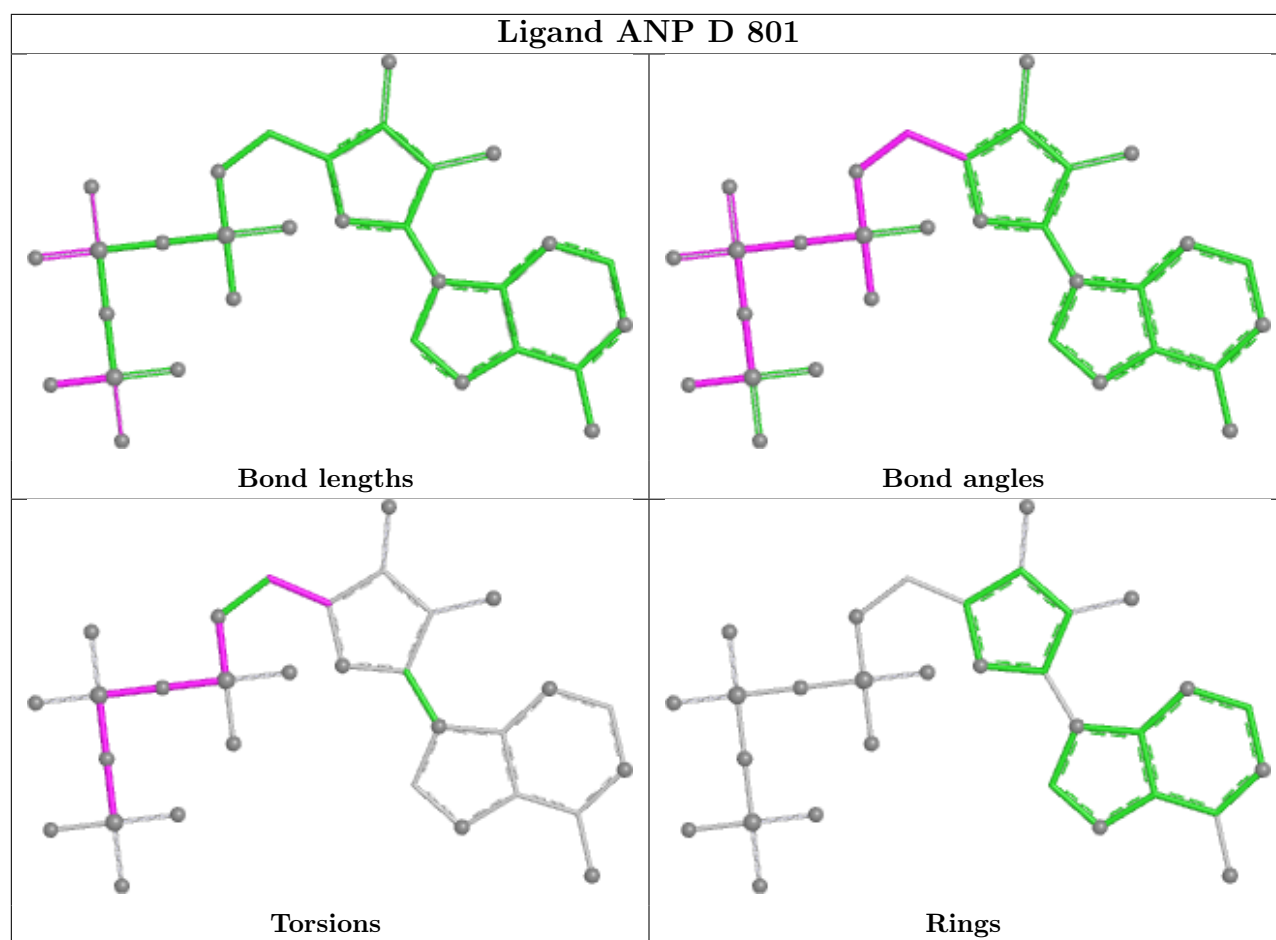
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ANP	1	0
2	C	801	ANP	1	0
2	D	801	ANP	3	0

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	365/502 (72%)	0.12	6 (1%)	70 52	39, 75, 149, 189	1 (0%)
1	B	472/502 (94%)	-0.02	5 (1%)	78 60	35, 67, 113, 170	1 (0%)
1	C	471/502 (93%)	0.09	5 (1%)	78 60	36, 81, 144, 195	1 (0%)
1	D	449/502 (89%)	0.12	12 (2%)	56 37	35, 78, 144, 193	0
All	All	1757/2008 (87%)	0.07	28 (1%)	70 52	35, 74, 141, 195	3 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	TYR	4.4
1	C	191	ALA	4.1
1	C	193	ALA	3.3
1	D	411	ILE	3.1
1	C	192	GLU	3.0
1	D	361	SER	2.8
1	A	438	ALA	2.8
1	B	490	MET	2.6
1	C	376	ALA	2.5
1	B	70	PRO	2.5
1	B	191	ALA	2.4
1	D	193	ALA	2.4
1	D	497	ILE	2.3
1	A	436	LYS	2.3
1	B	193	ALA	2.3
1	D	456	THR	2.3
1	D	335	ALA	2.3
1	A	408	SER	2.3
1	B	119	ASN	2.3
1	C	187	LEU	2.2
1	A	407	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	298	ILE	2.1
1	D	408	SER	2.1
1	D	336	PRO	2.1
1	D	184	LEU	2.1
1	D	192	GLU	2.1
1	D	295	LEU	2.1
1	A	352	MET	2.1

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](#)

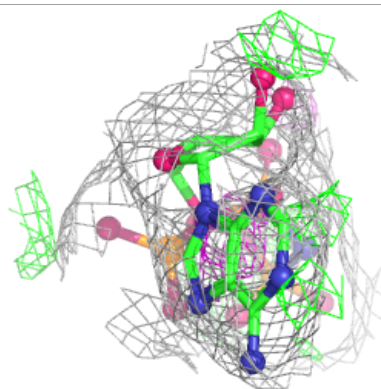
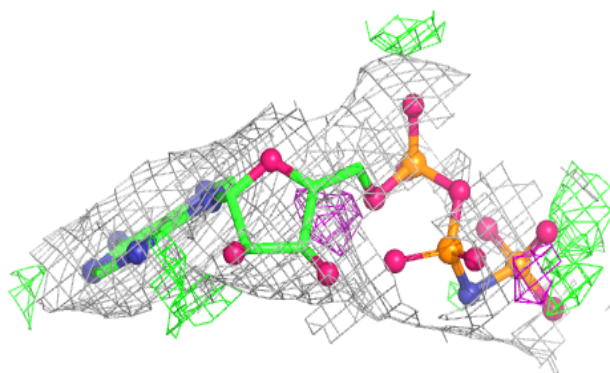
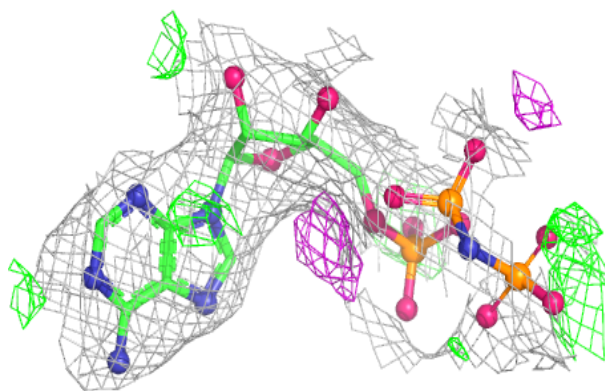
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	C	802	1/1	0.86	0.09	98,98,98,98	0
3	MG	D	802	1/1	0.89	0.13	215,215,215,215	0
3	MG	A	802	1/1	0.90	0.12	42,42,42,42	0
3	MG	B	802	1/1	0.92	0.08	36,36,36,36	0
2	ANP	D	801	31/31	0.94	0.09	53,59,87,108	0
2	ANP	C	801	31/31	0.96	0.08	42,48,74,125	0
2	ANP	A	801	31/31	0.96	0.07	37,40,53,99	0
2	ANP	B	801	31/31	0.97	0.07	13,51,55,129	0

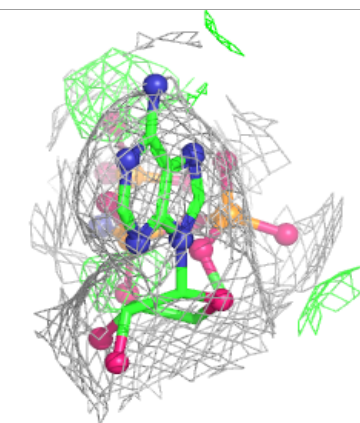
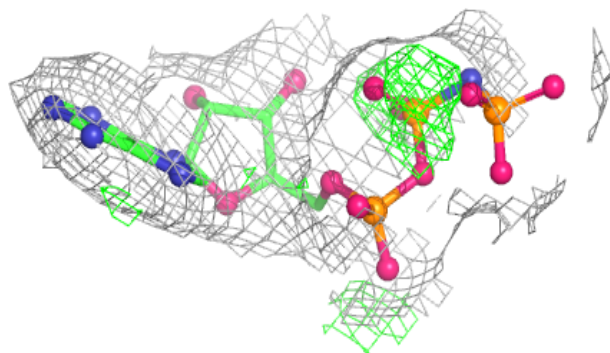
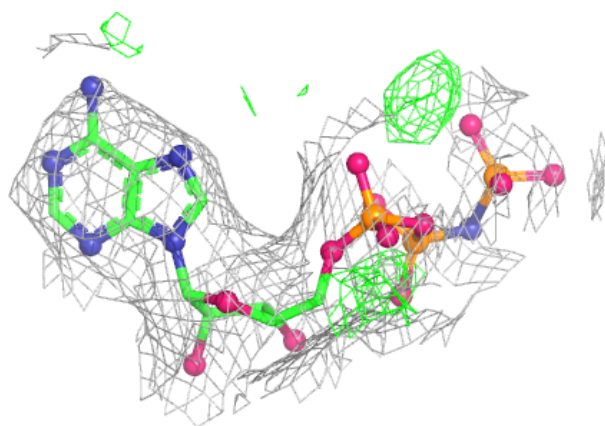
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP D 801:

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

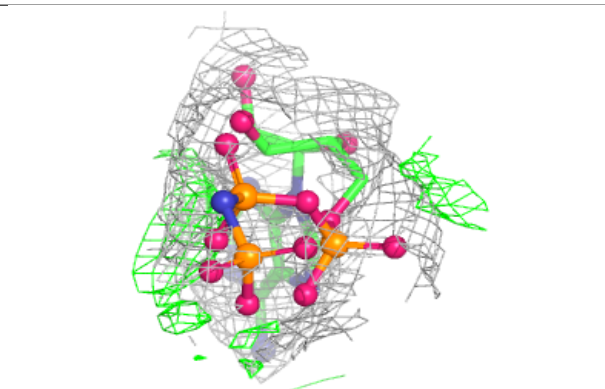
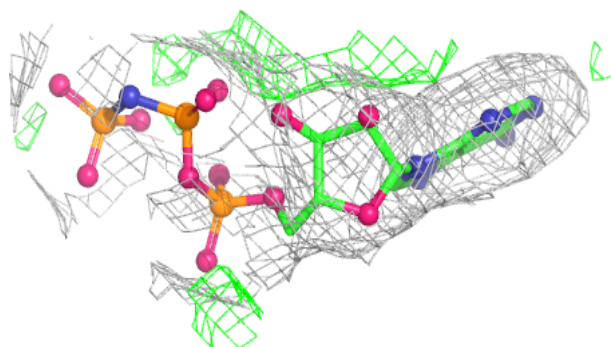
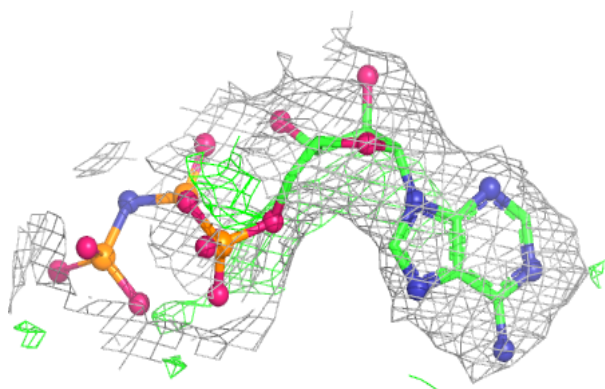
**Electron density around ANP C 801:**

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

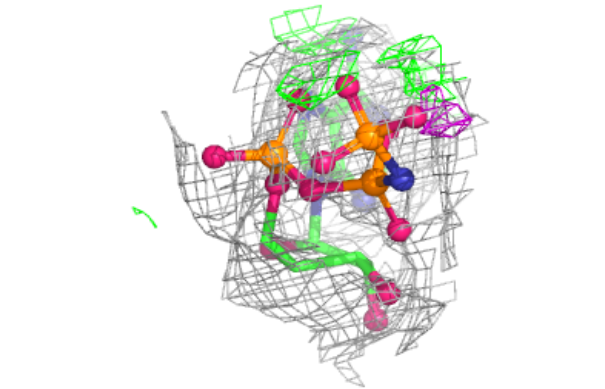
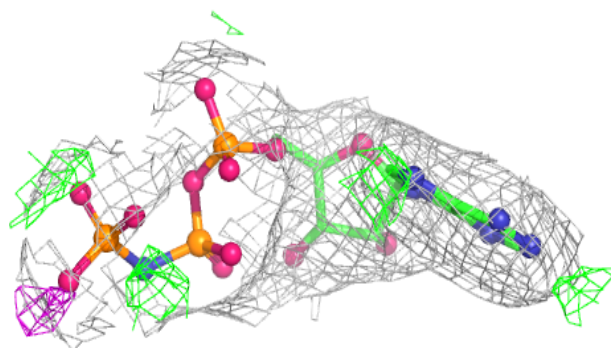
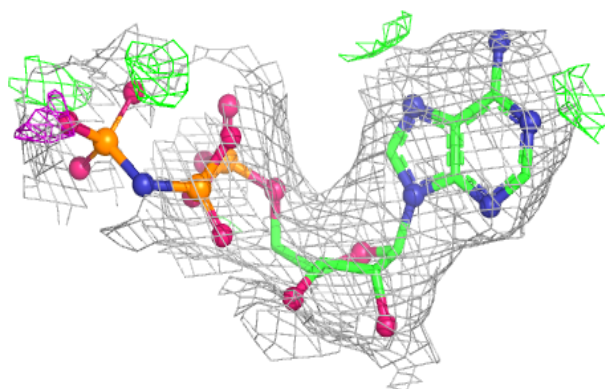


Electron density around ANP A 801:

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

**Electron density around ANP B 801:**

$2mF_o-DF_c$ (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.