Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 05:11 PM EDT

PDB ID	:	4Z1I
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 (i) 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 (i)) were used in the production of this report:

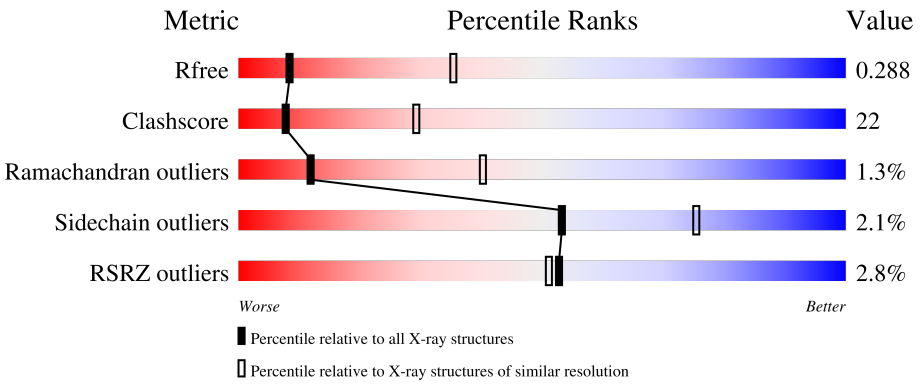
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	4% 45% 25% • • 27%
1	B	502	% 65% 27% • • 6%
1	C	502	2% 61% 29% • • 6%
1	D	502	3% 59% 27% • • 11%

2 Entry composition (i)

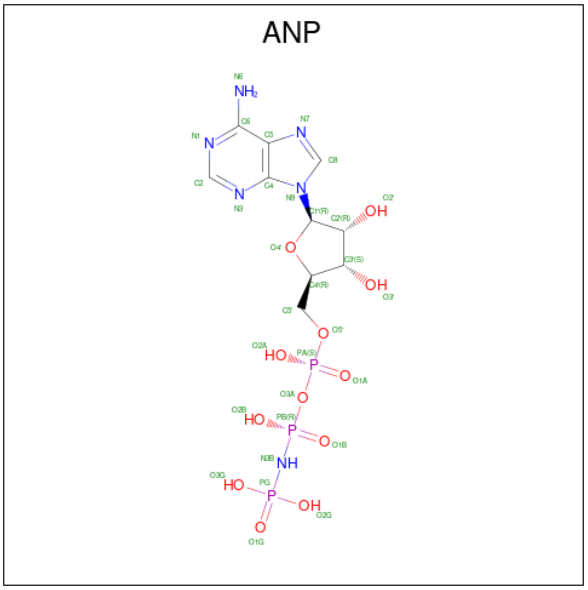
There are 3 unique types of molecules in this entry. The entry contains 14236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

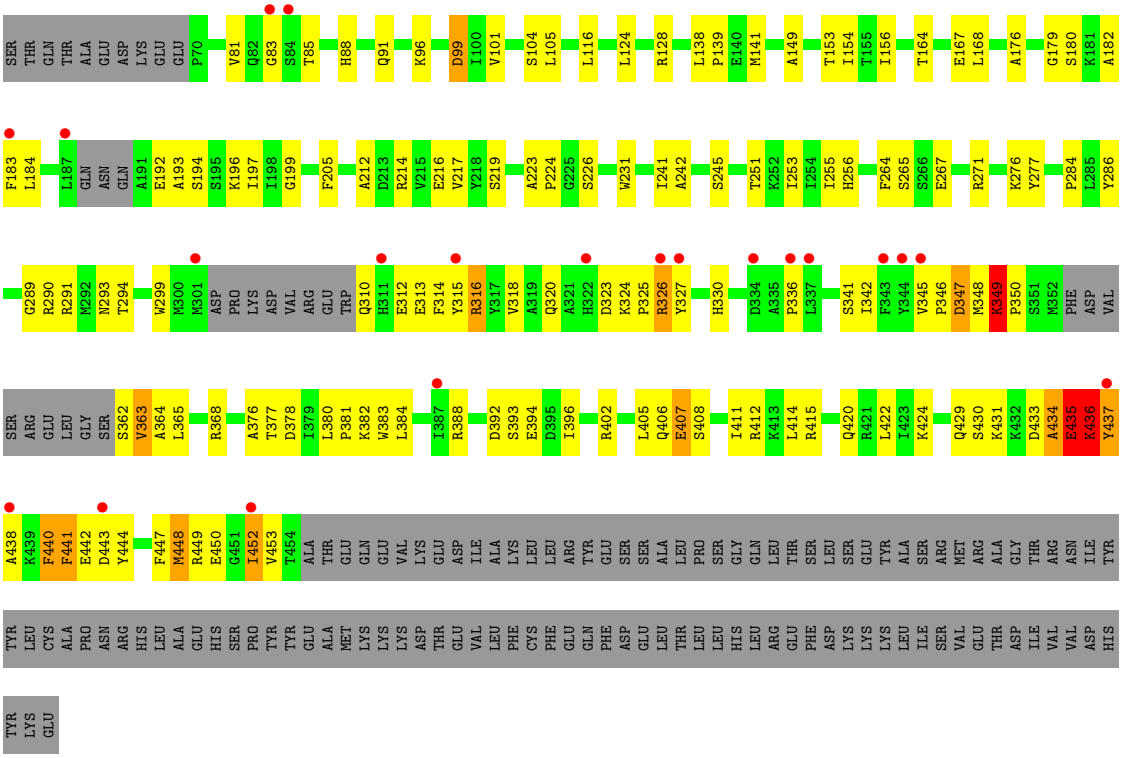
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
			Total	Mg		
3	B	1	1	1	0	0
			Total	Mg		
3	C	1	1	1	0	0
			Total	Mg		
3	D	1	1	1	0	0

3 Residue-property plots (i)

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.

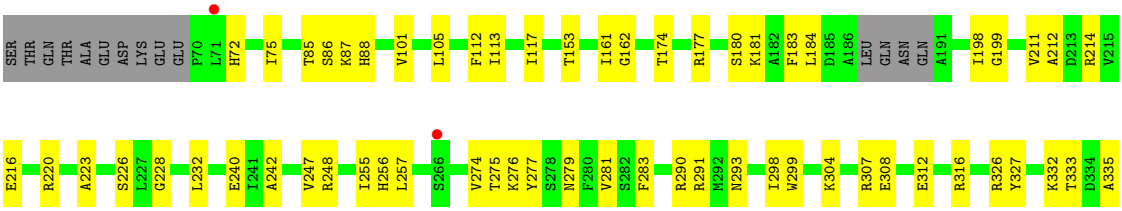
• Molecule 1: Heat shock protein 75 kDa, mitochondrial

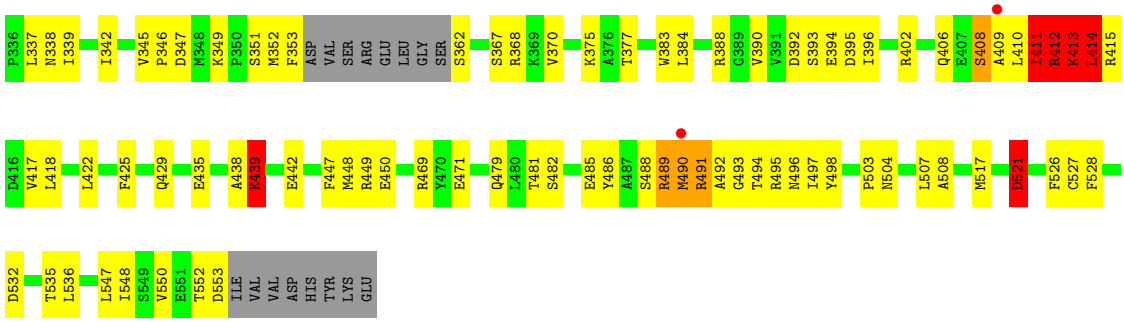
Chain A:



• Molecule 1: Heat shock protein 75 kDa, mitochondrial

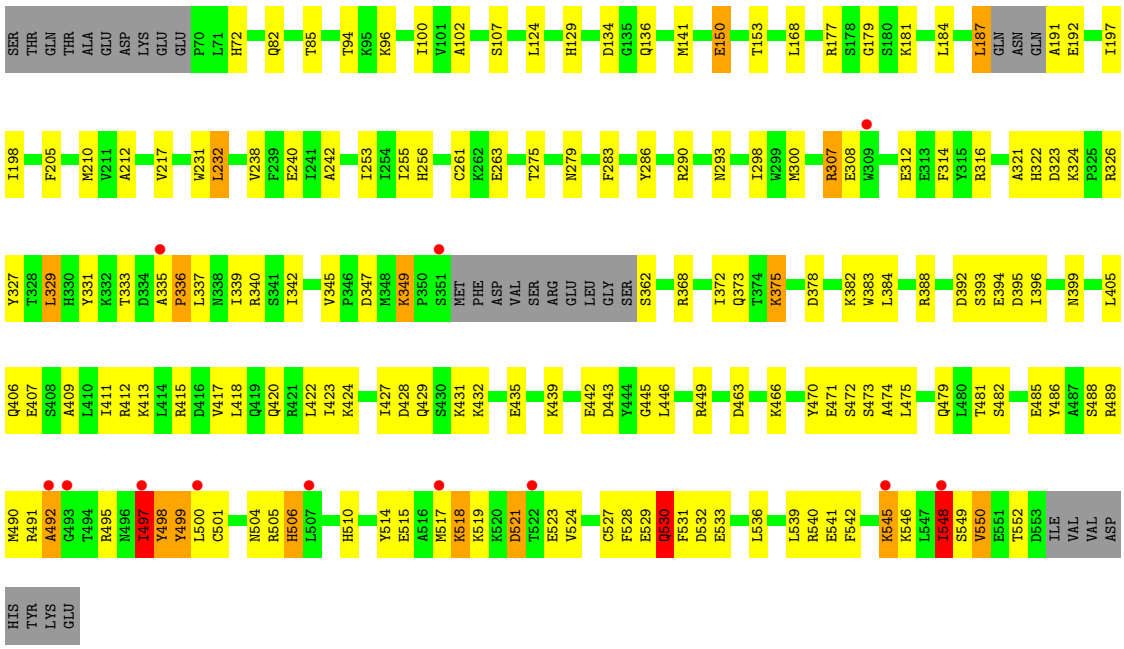
Chain B:





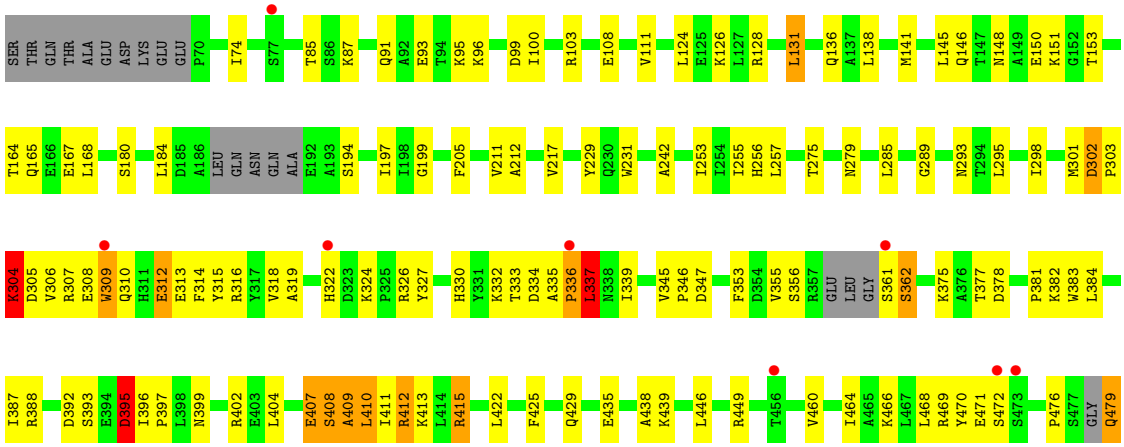
• Molecule 1: Heat shock protein 75 kDa, mitochondrial

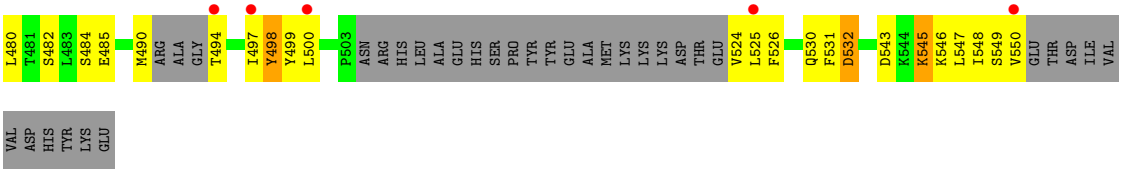
Chain C:



• Molecule 1: Heat shock protein 75 kDa, mitochondrial

Chain D:




L480
T481
S482
L483
S484
E485
M490
ARG
ALA
GLY
T494
I497
Y498
Y499
L500
P503
ASN
ARG
HIS
LEU
ALA
GLU
HIS
SER
PRO
TYR
TYR
GLU
ALA
MET
LYS
LYS
LYS
ASP
THR
GLU
V524
L525
F526
Q530
F531
D532
D543
K544
K545
K546
L547
I548
S549
V550
GLU
THR
ASP
ILE
VAL
VAL
ASP
HIS
TYR
LYS
GLU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.97 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.220 , 0.285 0.227 , 0.288	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)	0.32 , 63.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.89	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.42	0/2963	0.80	9/3987 (0.2%)
1	B	0.39	0/3871	0.75	6/5213 (0.1%)
1	C	0.52	6/3859 (0.2%)	0.85	16/5198 (0.3%)
1	D	0.48	3/3677 (0.1%)	0.82	20/4948 (0.4%)
All	All	0.46	9/14370 (0.1%)	0.81	51/19346 (0.3%)

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	D	498	TYR	CD1-CE1	-12.09	1.21	1.39
1	C	499	TYR	CD1-CE1	9.66	1.53	1.39
1	C	498	TYR	CD2-CE2	-8.35	1.26	1.39
1	C	498	TYR	CE2-CZ	-7.96	1.28	1.38
1	C	498	TYR	CB-CG	-7.18	1.40	1.51
1	D	498	TYR	CE1-CZ	-6.37	1.30	1.38
1	D	309	TRP	CB-CG	-6.33	1.38	1.50
1	C	498	TYR	CD1-CE1	-5.62	1.30	1.39
1	C	550	VAL	CA-CB	5.30	1.65	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	191	ALA	N-CA-C	12.19	143.91	111.00
1	B	414	LEU	CA-CB-CG	11.32	141.33	115.30
1	B	439	LYS	CD-CE-NZ	10.06	134.85	111.70
1	B	411	ILE	CG1-CB-CG2	-9.64	90.18	111.40
1	C	192	GLU	N-CA-CB	-9.34	93.79	110.60
1	C	335	ALA	C-N-CD	-8.77	101.31	120.60
1	A	347	ASP	CB-CG-OD1	-8.49	110.66	118.30
1	D	395	ASP	CB-CG-OD1	7.93	125.43	118.30
1	D	309	TRP	CA-CB-CG	7.72	128.38	113.70
1	C	498	TYR	C-N-CA	7.52	140.50	121.70
1	D	302	ASP	CB-CG-OD1	7.05	124.65	118.30
1	D	415	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	D	410	LEU	CB-CG-CD2	6.58	122.18	111.00
1	A	436	LYS	N-CA-C	6.48	128.50	111.00
1	A	349	LYS	C-N-CD	6.43	141.91	128.40
1	C	497	ILE	CB-CA-C	-6.42	98.76	111.60
1	D	498	TYR	CZ-CE2-CD2	-6.14	114.27	119.80
1	A	448	MET	C-N-CA	-6.10	106.45	121.70
1	A	349	LYS	C-N-CA	-6.08	96.45	122.00
1	B	521	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	518	LYS	C-N-CA	-5.91	106.92	121.70
1	A	99	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	C	498	TYR	N-CA-C	5.85	126.80	111.00
1	D	304	LYS	CD-CE-NZ	-5.84	98.27	111.70
1	C	499	TYR	CB-CG-CD1	5.81	124.49	121.00
1	A	347	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	335	ALA	C-N-CA	5.77	146.22	122.00
1	D	532	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	C	446	LEU	CA-CB-CG	5.72	128.47	115.30
1	C	548	ILE	O-C-N	-5.70	113.58	122.70
1	D	498	TYR	C-N-CA	5.66	135.85	121.70
1	D	308	GLU	C-N-CA	-5.65	107.58	121.70
1	D	312	GLU	CA-CB-CG	5.63	125.80	113.40
1	A	435	GLU	C-N-CA	5.59	135.69	121.70
1	D	312	GLU	N-CA-CB	-5.57	100.58	110.60
1	D	131	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	C	498	TYR	N-CA-CB	-5.46	100.77	110.60
1	D	545	LYS	N-CA-C	-5.34	96.59	111.00
1	D	131	LEU	CB-CG-CD1	5.29	119.99	111.00
1	C	499	TYR	O-C-N	-5.25	114.30	122.70
1	D	498	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	C	232	LEU	CA-CB-CG	5.22	127.32	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	489	ARG	N-CA-C	5.18	125.00	111.00
1	D	498	TYR	CE1-CZ-OH	-5.18	106.12	120.10
1	D	302	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	532	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	491	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	C	548	ILE	C-N-CA	-5.09	108.98	121.70
1	D	304	LYS	CB-CG-CD	5.05	124.73	111.60
1	C	191	ALA	CB-CA-C	-5.04	102.54	110.10
1	A	99	ASP	CB-CG-OD2	5.01	122.81	118.30

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	147	0
1	B	3798	0	3799	145	0
1	C	3787	0	3793	175	0
1	D	3612	0	3625	170	0
2	A	31	0	13	1	0
2	B	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	619	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (619) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:499:TYR:CD1	1:C:536:LEU:HD13	2.17	0.79
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:SER:OG	1:B:352:MET:N	2.20	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: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: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
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:C:490:MET:C	1:C:491:ARG:HG3	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:321:ALA:C	1:C:322:HIS:HD2	1.99	0.66
1:D:212:ALA:HB2	1:D:255:ILE:HG23	1.78	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
1:B:413:LYS:HZ1	1:B:415:ARG:HG2	1.61	0.66
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:D:302:ASP:OD1	1:D:332:LYS:NZ	2.29	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:C:375:LYS:HG2	1:C:375:LYS:O	1.98	0.64
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: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: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:D:312:GLU:CD	1:D:316:ARG:HH12	2.01	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:335:ALA:O	1:D:336:PRO:C	2.38	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:A:407:GLU:H	1:A:407:GLU:CD	2.06	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:348:MET:C	1:A:349:LYS:HD3	2.24	0.58
1:B:412:ARG:NH1	1:B:415:ARG:HH21	2.01	0.58
1:C:490:MET:C	1:C:491:ARG:CG	2.72	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: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:D:435:GLU:C	1:D:439:LYS:HZ2	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:515:GLU:HG3	1:C:518:LYS:HZ1	1.68	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:442:GLU:C	1:A:444:TYR:H	2.08	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: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: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:290:ARG:HD3	1:B:290:ARG:C	2.27	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:435:GLU:HG2	1:D:439:LYS:HZ2	1.72	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:B:469:ARG:NH1	1:B:482:SER:HG	2.06	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:349:LYS:HG3	1:A:443:ASP:CG	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:321:ALA:C	1:C:322:HIS:CD2	2.80	0.52
1:A:316:ARG:HH21	1:A:323:ASP:C	2.11	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
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: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:B:496:ASN:CG	1:B:548:ILE:HD13	2.30	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:223:ALA:O	1:A:226:SER:OG	2.19	0.51
1:C:420:GLN:O	1:C:424:LYS:HG3	2.11	0.51
1:D:96:LYS:O	1:D:100:ILE:HG13	2.11	0.51
1:B:307:ARG:CG	1:B:308:GLU:N	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:LYS:HA	1:B:442:GLU:HB2	1.93	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
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: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: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:A:442:GLU:C	1:A:444:TYR:N	2.66	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:O	1:C:96:LYS:CE	2.60	0.48
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: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:473:SER:OG	1:C:523:GLU:OE1	2.31	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
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:476:PRO:HD2	1:D:479:GLN:HB2	1.95	0.48
1:D:532:ASP:OD1	1:D:532:ASP:N	2.45	0.48
1:A:214:ARG:HH21	1:A:256:HIS:CE1	2.32	0.48
1:A:440:PHE:O	1:A:441:PHE:C	2.50	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: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:A:276:LYS:HD3	1:A:277:TYR:CZ	2.49	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:301:MET:C	1:D:332:LYS:HZ1	2.19	0.47
1:C:399:ASN:HA	1:C:406:GLN:HG3	1.96	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:A:407:GLU:CD	1:A:407:GLU:N	2.69	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:550:VAL:C	1:C:552:THR:H	2.18	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:C:530:GLN:CD	1:C:530:GLN:O	2.54	0.46
1:D:312:GLU:CD	1:D:316:ARG:NH1	2.67	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: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: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
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:312:GLU:O	1:D:315:TYR:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:293:ASN:OD1	1:B:293:ASN:N	2.49	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:375:LYS:HD2	1:D:375:LYS:HA	1.44	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: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:A:310:GLN:C	1:A:312:GLU:H	2.20	0.45
1:B:418:LEU:O	1:B:422:LEU:N	2.43	0.45
1:D:395:ASP:C	1:D:395:ASP:OD1	2.54	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:D:399:ASN:HB3	1:D:404:LEU:HB3	2.00	0.44
1:C:168:LEU:HD13	1:C:231:TRP:HB2	1.99	0.44
1:C:321:ALA:O	1:C:322:HIS:HD2	1.99	0.44
1:A:284:PRO:HB3	1:A:291:ARG:HH12	1.82	0.44
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: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
2:A:801:ANP:O2B	2:A:801:ANP:O3'	2.24	0.44
1:B:198:ILE:HA	1:B:368:ARG:HD3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:316:ARG:HH12	1:C:323:ASP:C	2.20	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:C:261:CYS:C	1:C:263:GLU:N	2.71	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
1:C:124:LEU:HD22	1:C:141:MET:HB3	2.00	0.43
1:D:335:ALA:C	1:D:337:LEU:N	2.71	0.43
1:A:347:ASP:OD1	1:A:347:ASP:N	2.50	0.43
1:A:442:GLU:OE2	1:A:442:GLU:O	2.37	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:314:PHE:O	1:D:318:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ASP:CG	1:D:103:ARG:HH12	2.21	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:A:412:ARG:C	1:A:415:ARG:HB3	2.38	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:A:310:GLN:C	1:A:312:GLU:N	2.72	0.43
1:B:212:ALA:HB2	1:B:255:ILE:HG23	1.99	0.43
1:C:500:LEU:HD12	1:C:550:VAL:CG2	2.49	0.43
1:A:434:ALA:C	1:A:436:LYS:HG3	2.39	0.42
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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:99:ASP:OD1	1:D:103:ARG:NH2	2.54	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:530:GLN:C	1:C:532:ASP:H	2.20	0.41
1:D:356:SER:O	1:D:356:SER:OG	2.37	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:86:SER:HG	1:B:88:HIS:CE1	2.38	0.41
1:B:411:ILE:HG22	1:B:415:ARG:HE	1.84	0.41
1:C:422:LEU:HA	1:C:422:LEU:HD23	1.84	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:B:408:SER:O	1:B:409:ALA:C	2.59	0.41
1:C:298:ILE:HG22	1:C:342:ILE:HD11	2.03	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:150:GLU:CD	1:D:150:GLU:H	2.25	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:A:341:SER:C	1:A:342:ILE:HD12	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:378:ASP:CG	1:A:415:ARG:HH21	2.24	0.40
1:A:447:PHE:C	1:A:450:GLU:HB3	2.41	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:B:112:PHE:CG	1:B:113:ILE:N	2.89	0.40
1:D:312:GLU:CD	1:D:316:ARG:HH22	2.18	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	357/502 (71%)	310 (87%)	35 (10%)	12 (3%)	3 22
1	B	466/502 (93%)	433 (93%)	30 (6%)	3 (1%)	25 57
1	C	465/502 (93%)	442 (95%)	19 (4%)	4 (1%)	17 48
1	D	437/502 (87%)	412 (94%)	21 (5%)	4 (1%)	17 48
All	All	1725/2008 (86%)	1597 (93%)	105 (6%)	23 (1%)	12 40

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 (i)

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%)	308 (97%)	10 (3%)	40	67
1	B	415/443 (94%)	409 (99%)	6 (1%)	67	82
1	C	414/443 (94%)	405 (98%)	9 (2%)	52	74
1	D	398/443 (90%)	391 (98%)	7 (2%)	59	78
All	All	1545/1772 (87%)	1513 (98%)	32 (2%)	53	75

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	128	ARG
1	A	196	LYS
1	A	216	GLU
1	A	316	ARG
1	A	326	ARG
1	A	349	LYS
1	A	431	LYS
1	A	440	PHE
1	A	448	MET
1	B	87	LYS
1	B	408	SER
1	B	412	ARG
1	B	439	LYS
1	B	490	MET
1	B	527	CYS
1	C	150	GLU
1	C	187	LEU
1	C	329	LEU
1	C	349	LYS
1	C	375	LYS
1	C	495	ARG
1	C	506	HIS
1	C	545	LYS
1	C	546	LYS
1	D	295	LEU
1	D	304	LYS
1	D	337	LEU
1	D	395	ASP
1	D	408	SER
1	D	412	ARG
1	D	479	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	399	ASN
1	C	322	HIS
1	D	136	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	801	3	29,33,33	2.13	6 (20%)	31,52,52	1.05	2 (6%)
2	ANP	B	801	1,3	29,33,33	1.11	4 (13%)	31,52,52	1.33	3 (9%)
2	ANP	D	801	1,3	29,33,33	2.04	4 (13%)	31,52,52	2.73	7 (22%)
2	ANP	C	801	1,3	29,33,33	1.19	4 (13%)	31,52,52	1.07	3 (9%)

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	A	801	3	-	6/14/38/38	0/3/3/3
2	ANP	B	801	1,3	-	3/14/38/38	0/3/3/3
2	ANP	D	801	1,3	-	10/14/38/38	0/3/3/3
2	ANP	C	801	1,3	-	9/14/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	PG-O1G	7.58	1.58	1.46
2	D	801	ANP	PG-O1G	7.52	1.58	1.46
2	A	801	ANP	PB-O1B	6.36	1.56	1.46
2	D	801	ANP	PB-O1B	5.56	1.55	1.46
2	C	801	ANP	PB-O3A	-3.21	1.55	1.59
2	D	801	ANP	PB-O2B	-2.89	1.49	1.56
2	A	801	ANP	PB-O2B	-2.64	1.49	1.56
2	A	801	ANP	PG-N3B	2.53	1.70	1.63
2	A	801	ANP	PG-O2G	-2.52	1.50	1.56
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	C	801	ANP	PG-O1G	2.46	1.50	1.46
2	B	801	ANP	PG-O1G	2.45	1.50	1.46
2	B	801	ANP	PB-O3A	-2.41	1.56	1.59
2	D	801	ANP	PG-O2G	-2.35	1.50	1.56
2	C	801	ANP	PB-O1B	2.28	1.49	1.46
2	A	801	ANP	PB-O3A	-2.17	1.56	1.59
2	B	801	ANP	PB-O1B	2.14	1.49	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	ANP	O1G-PG-N3B	-12.01	94.08	111.77
2	D	801	ANP	PB-O3A-PA	-5.19	114.34	132.62
2	B	801	ANP	PB-O3A-PA	-4.75	115.89	132.62
2	D	801	ANP	O1B-PB-N3B	-4.66	104.91	111.77
2	C	801	ANP	PB-O3A-PA	-4.04	118.40	132.62
2	B	801	ANP	O1B-PB-N3B	-3.58	106.50	111.77
2	A	801	ANP	PB-O3A-PA	-3.53	120.18	132.62
2	D	801	ANP	O5'-C5'-C4'	3.04	119.45	108.99
2	D	801	ANP	PA-O5'-C5'	-2.48	107.13	121.68
2	C	801	ANP	O3G-PG-O1G	-2.39	107.45	113.45
2	B	801	ANP	C5-C6-N6	2.33	123.89	120.35
2	A	801	ANP	C5-C6-N6	2.26	123.79	120.35
2	D	801	ANP	C5-C6-N6	2.25	123.77	120.35
2	C	801	ANP	C5-C6-N6	2.22	123.73	120.35
2	D	801	ANP	O2B-PB-O3A	2.02	111.38	104.64

There are no chirality outliers.

All (28) 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-O1B
2	A	801	ANP	PA-O3A-PB-O2B
2	B	801	ANP	PB-N3B-PG-O1G
2	B	801	ANP	PA-O3A-PB-O1B
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	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'
2	C	801	ANP	PB-O3A-PA-O5'
2	D	801	ANP	PB-O3A-PA-O5'
2	C	801	ANP	C5'-O5'-PA-O3A
2	D	801	ANP	C5'-O5'-PA-O3A
2	C	801	ANP	C5'-O5'-PA-O2A
2	D	801	ANP	C5'-O5'-PA-O1A
2	D	801	ANP	C3'-C4'-C5'-O5'
2	C	801	ANP	PG-N3B-PB-O1B
2	D	801	ANP	PG-N3B-PB-O1B
2	C	801	ANP	O4'-C4'-C5'-O5'
2	C	801	ANP	C3'-C4'-C5'-O5'

There are no ring outliers.

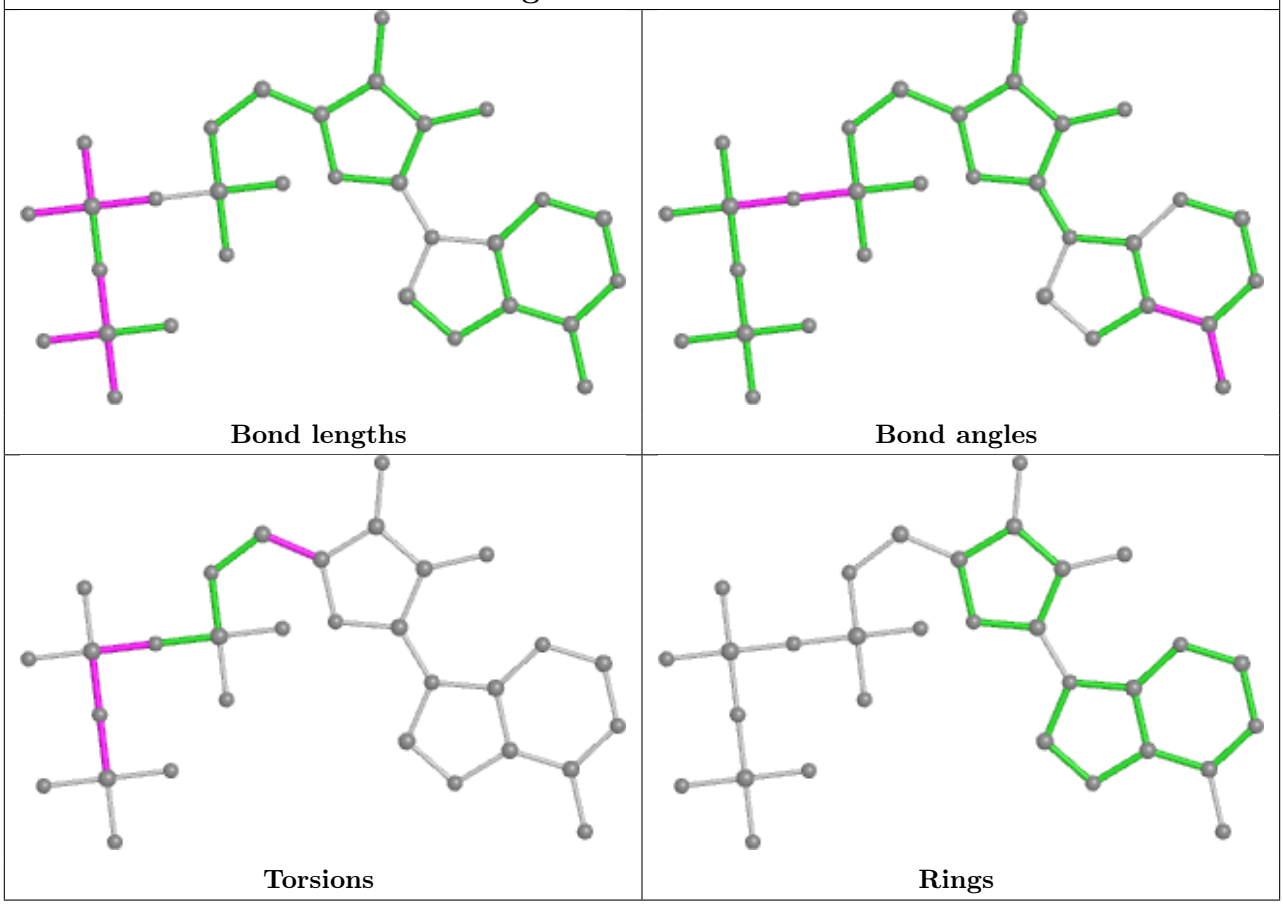
3 monomers are involved in 5 short contacts:

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

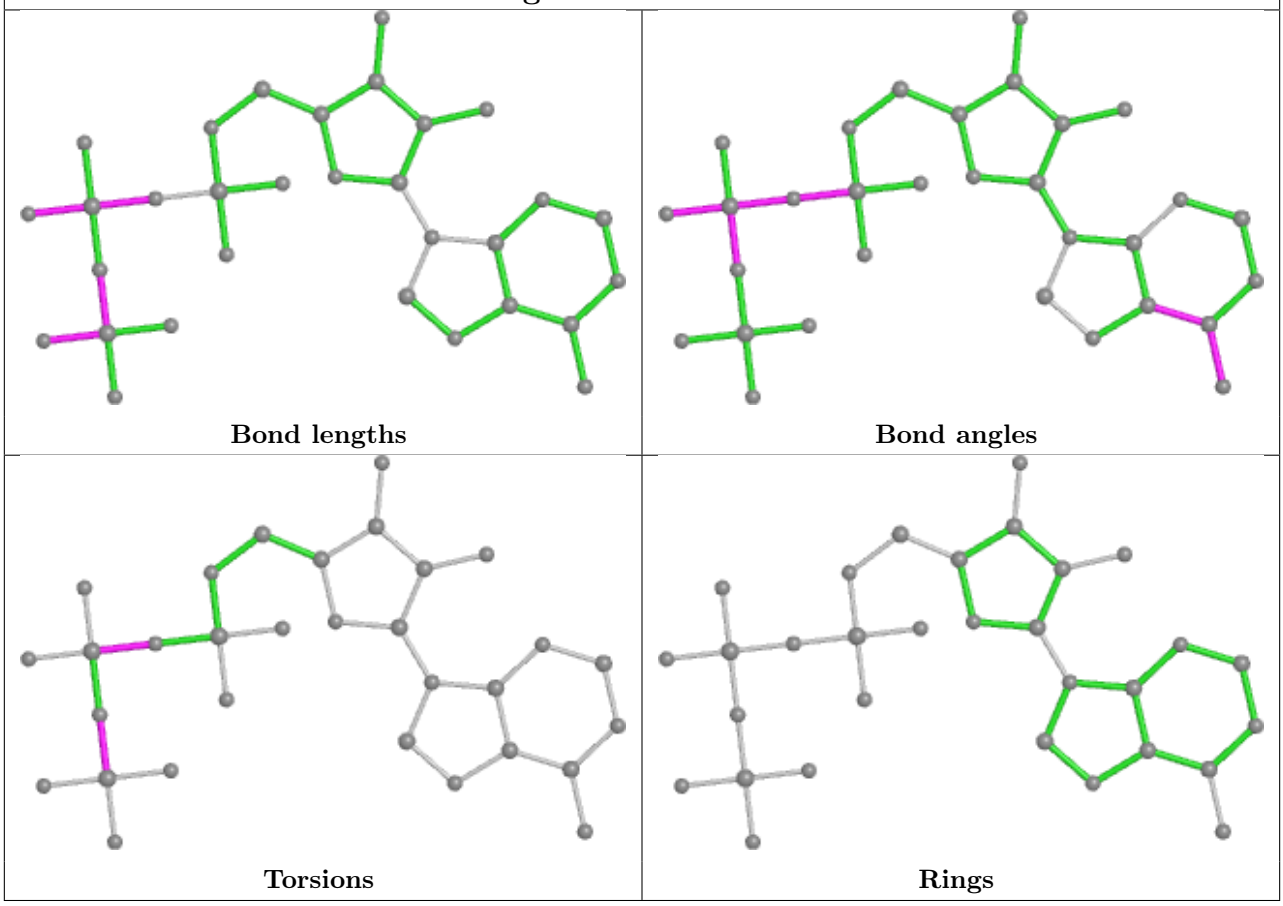
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

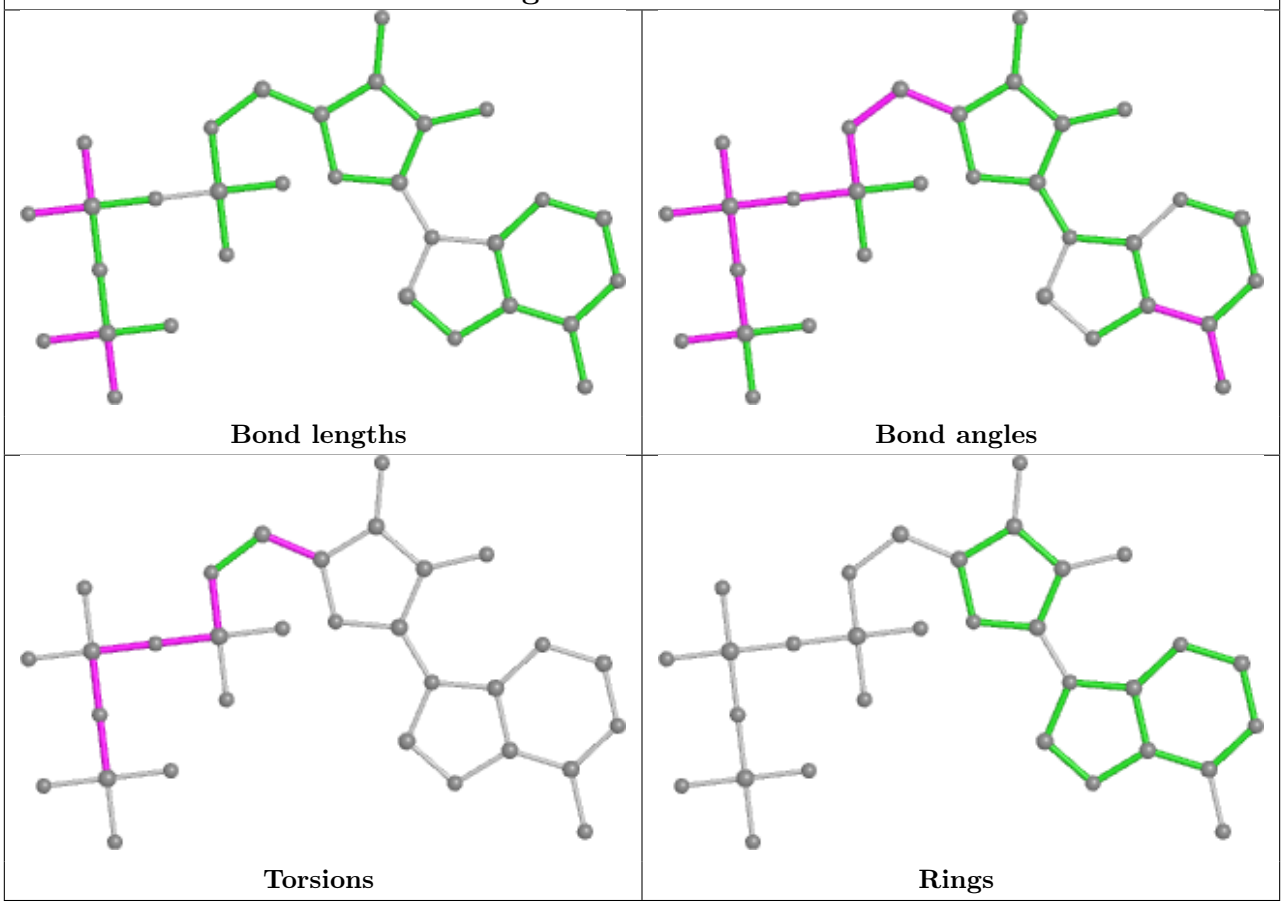
Ligand ANP A 801



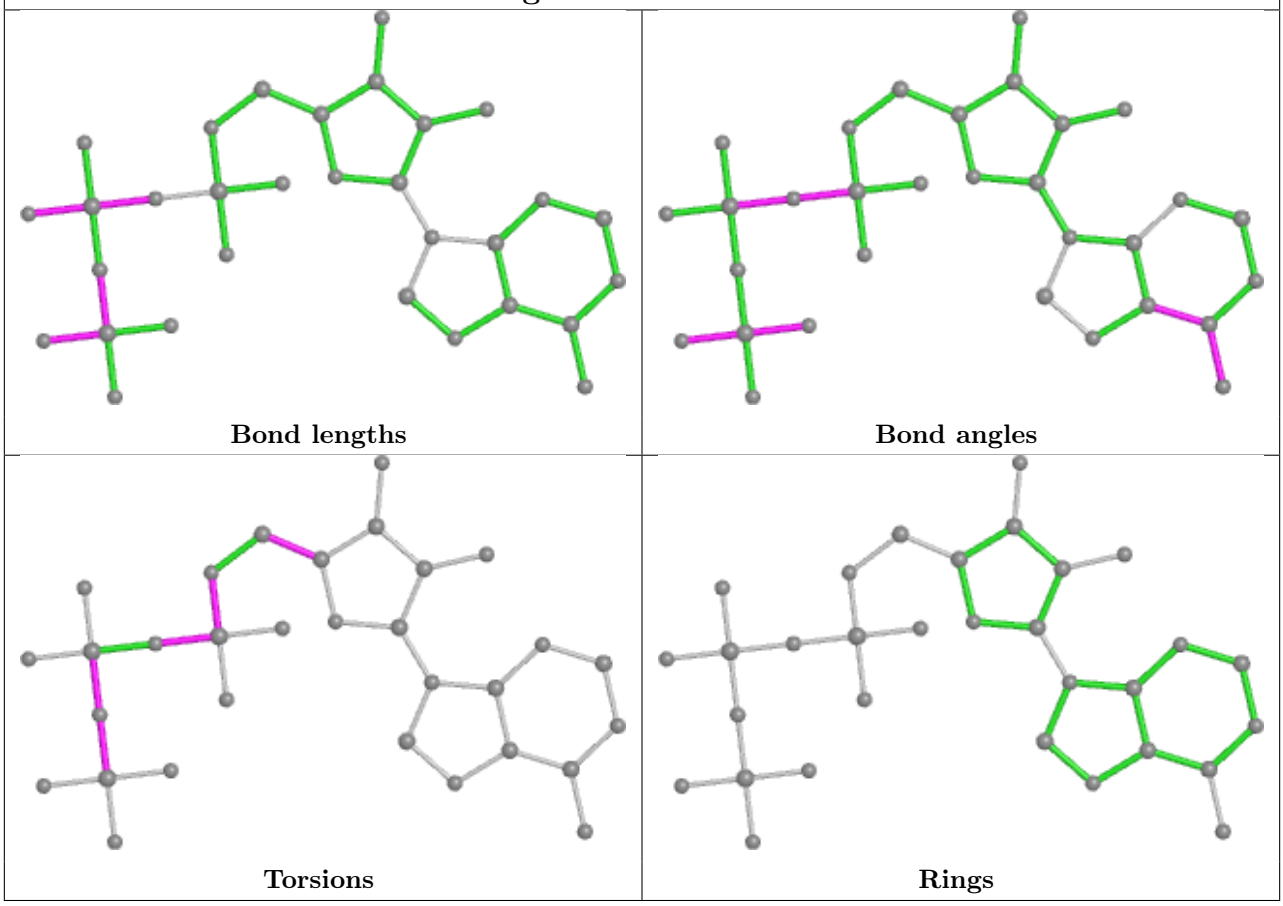
Ligand ANP B 801



Ligand ANP D 801



Ligand ANP C 801



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.19	21 (5%)	23	22	39, 75, 149, 189	1 (0%)
1	B	472/502 (94%)	0.04	4 (0%)	86	86	35, 67, 113, 170	1 (0%)
1	C	471/502 (93%)	0.11	12 (2%)	57	54	36, 81, 144, 195	1 (0%)
1	D	449/502 (89%)	0.11	13 (2%)	51	50	35, 78, 144, 193	0
All	All	1757/2008 (87%)	0.11	50 (2%)	53	51	35, 74, 141, 195	3 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	TYR	5.6
1	A	443	ASP	4.0
1	A	311	HIS	3.9
1	A	336	PRO	3.9
1	C	522	THR	3.6
1	C	309	TRP	3.5
1	C	493	GLY	3.5
1	D	336	PRO	3.4
1	B	71	LEU	3.4
1	D	497	ILE	3.4
1	A	387	ILE	3.3
1	C	492	ALA	3.3
1	A	83	GLY	3.2
1	C	517	MET	3.2
1	A	438	ALA	3.1
1	A	343	PHE	3.1
1	D	500	LEU	3.1
1	A	345	VAL	3.1
1	B	409	ALA	3.1
1	D	361	SER	2.9
1	C	507	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	337	LEU	2.8
1	B	490	MET	2.7
1	C	335	ALA	2.7
1	A	322	HIS	2.7
1	A	327	TYR	2.7
1	A	452	ILE	2.6
1	D	309	TRP	2.6
1	C	351	SER	2.6
1	C	545	LYS	2.6
1	D	525	LEU	2.5
1	A	344	TYR	2.5
1	D	550	VAL	2.4
1	D	322	HIS	2.4
1	D	472	SER	2.4
1	B	266	SER	2.3
1	D	494	THR	2.2
1	C	497	ILE	2.2
1	A	326	ARG	2.2
1	A	183	PHE	2.1
1	A	301	MET	2.1
1	A	187	LEU	2.1
1	C	548	ILE	2.0
1	A	84	SER	2.0
1	D	77	SER	2.0
1	A	334	ASP	2.0
1	D	456	THR	2.0
1	D	473	SER	2.0
1	A	315	TYR	2.0
1	C	500	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

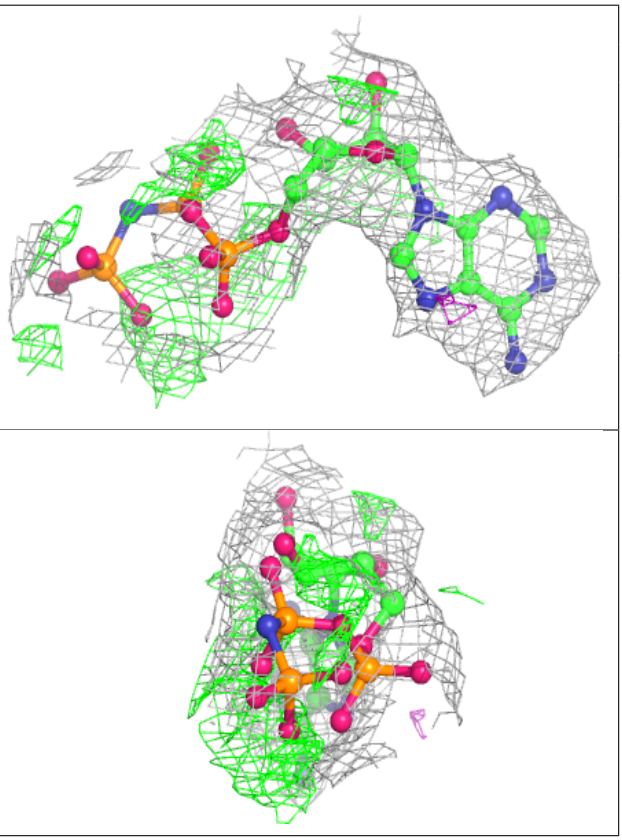
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.88	0.34	98,98,98,98	0
3	MG	B	802	1/1	0.89	0.31	36,36,36,36	0
3	MG	A	802	1/1	0.93	0.50	42,42,42,42	0
3	MG	D	802	1/1	0.94	0.18	215,215,215,215	0
2	ANP	A	801	31/31	0.95	0.26	37,40,53,99	0
2	ANP	D	801	31/31	0.95	0.25	53,59,87,108	0
2	ANP	C	801	31/31	0.96	0.24	42,48,74,125	0
2	ANP	B	801	31/31	0.97	0.24	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.

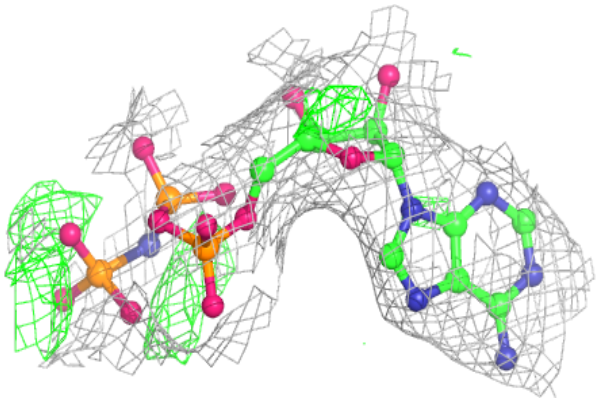
Electron density around ANP A 801:

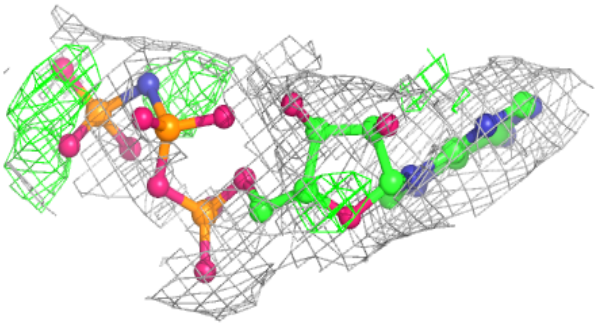
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

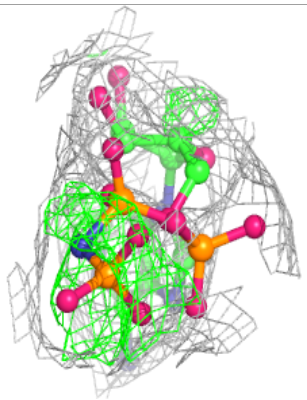


Electron density around ANP D 801:

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

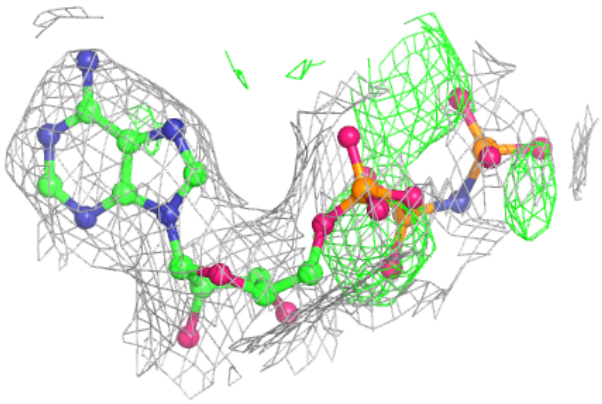


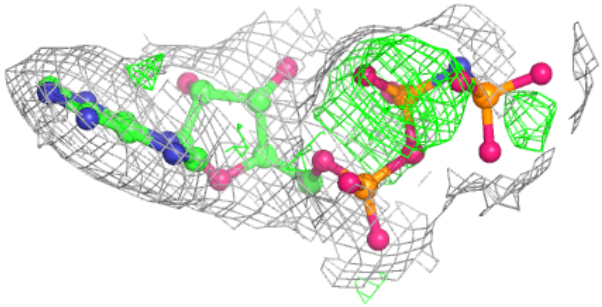


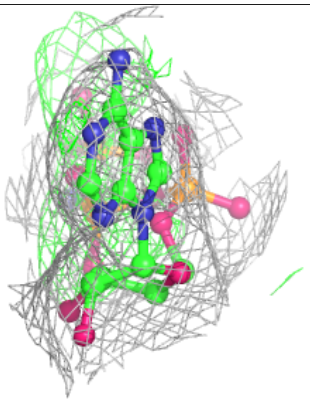


Electron density around ANP C 801:

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

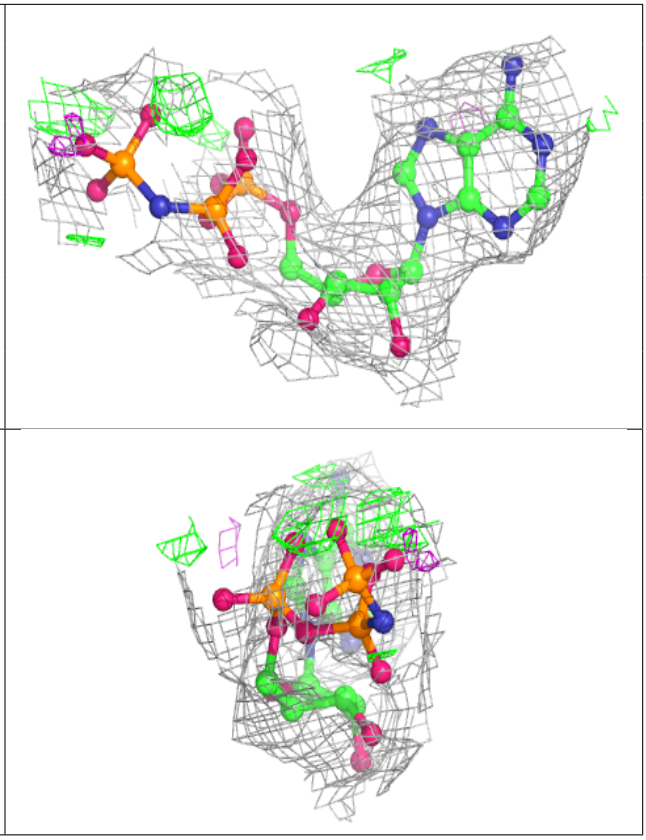






Electron density around ANP B 801:

$2mF_o$-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.