



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:16 AM UTC

PDB ID : 3BUZ / pdb_00003buz
Title : Crystal structure of ia-bTAD-actin complex
Authors : Tsuge, H.; Nagahama, M.; Oda, M.; Iwamoto, S.; Utsunomiya, H.; Marquez, V.E.; Katunuma, N.; Nishizawa, M.; Sakurai, J.
Deposited on : 2008-01-04
Resolution : 2.81 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

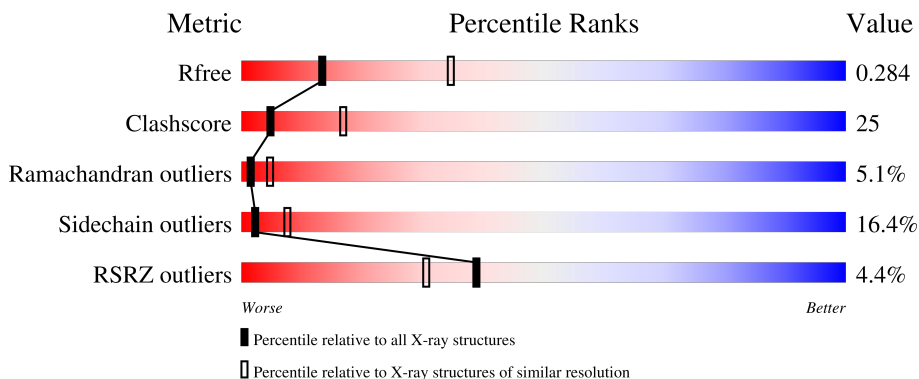
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	413	4% 47% 37% 14% .
2	B	375	4% 44% 38% 13% ..

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6364 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.

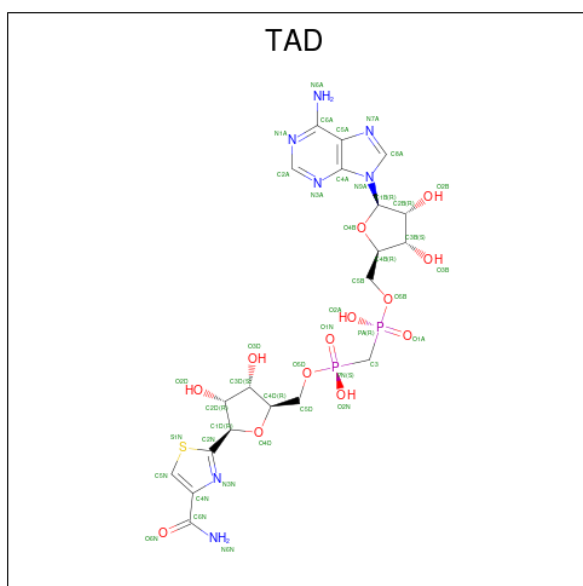
- Molecule 1 is a protein called Iota toxin component Ia.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3364	2146	553	662	3			

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	360	Total	C	N	O	S	0	0	0
			2817	1785	474	539	19			

- Molecule 3 is BETA-METHYLENE-THIAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (CCD ID: TAD) (formula: $C_{20}H_{27}N_7O_{13}P_2S$).

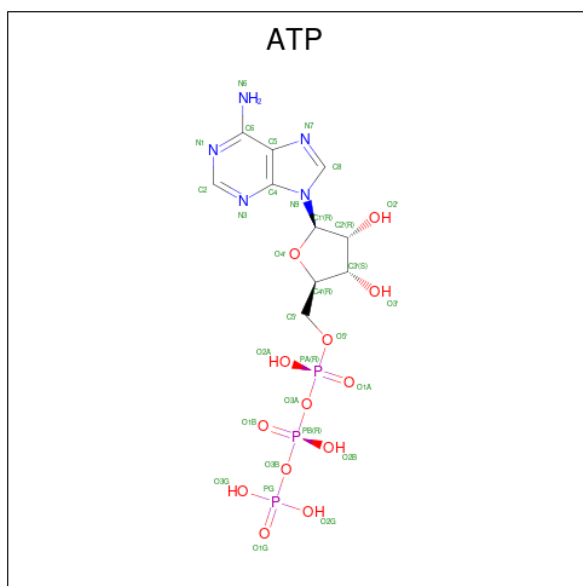


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			43	20	7	13	2		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

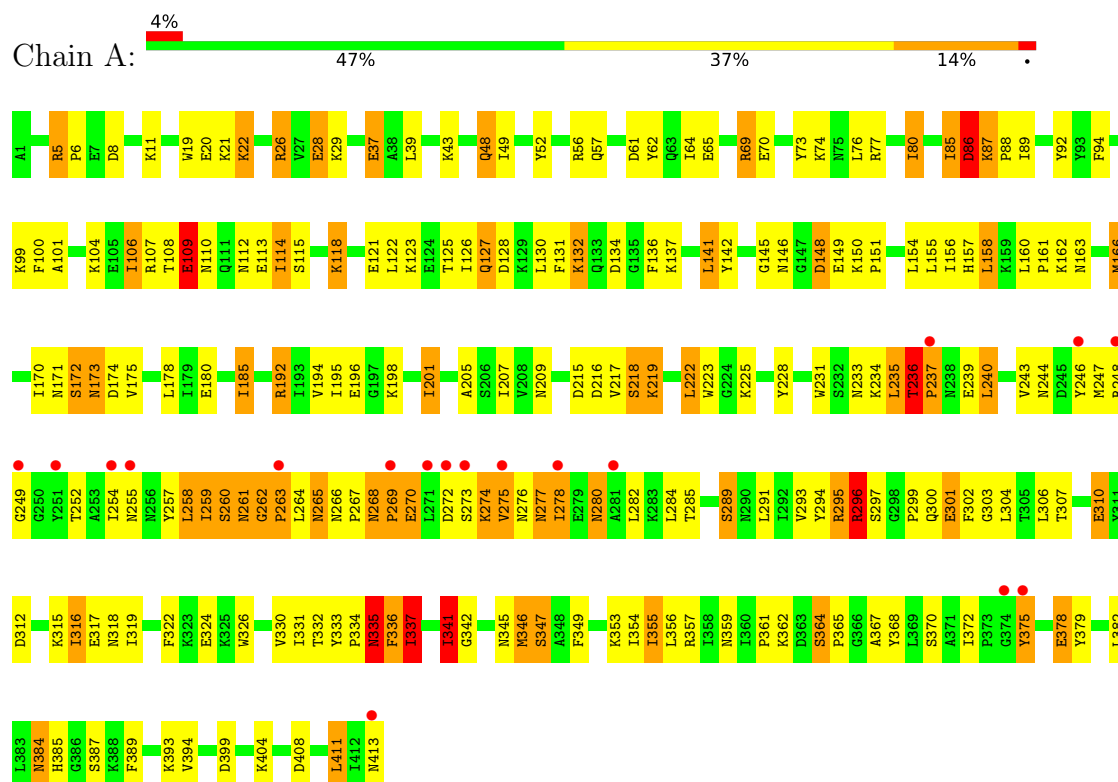
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	41	Total	O	0	0
			41	41		
7	B	38	Total	O	0	0
			38	38		

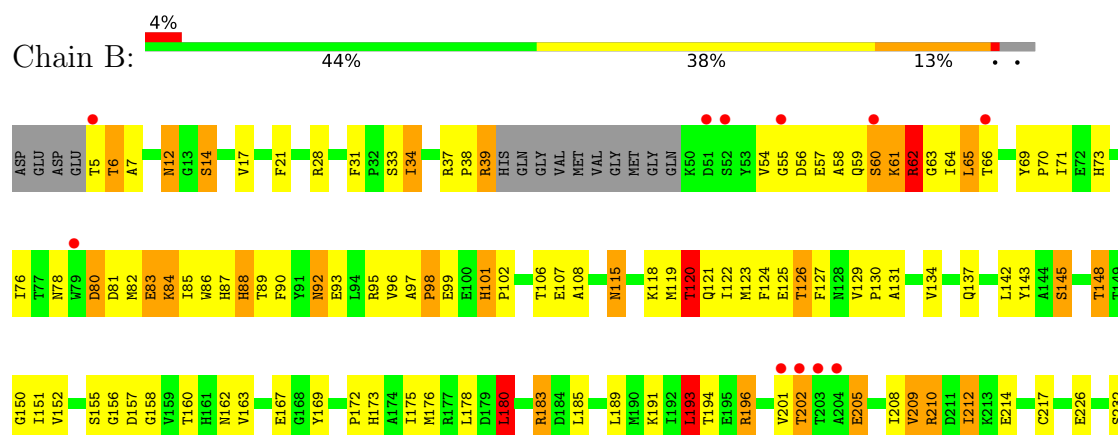
3 Residue-property plots [i](#)

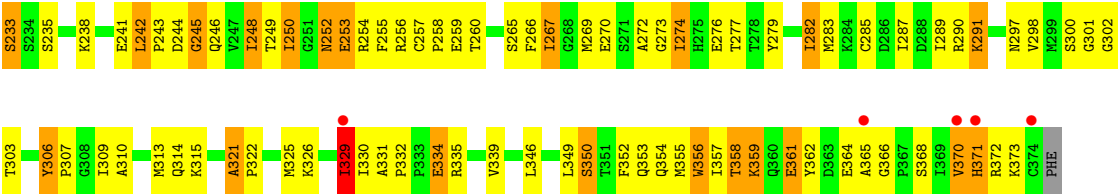
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: Actin, alpha skeletal muscle





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.01Å 126.34Å 147.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.69 – 2.81 36.69 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.69-2.81) 99.1 (36.69-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.02 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.298 0.218 , 0.284	Depositor DCC
R_{free} test set	1333 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6364	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: TAD, CA, ATP, LAR

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	1.30	6/3433 (0.2%)	1.46	45/4637 (1.0%)
2	B	1.30	9/2877 (0.3%)	1.42	32/3899 (0.8%)
All	All	1.30	15/6310 (0.2%)	1.44	77/8536 (0.9%)

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	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	ASP	C-N	11.04	1.47	1.33
2	B	289	ILE	CA-CB	-9.13	1.44	1.54
1	A	11	LYS	C-N	-8.13	1.23	1.33
1	A	341	ILE	CA-CB	7.43	1.63	1.54
1	A	86	ASP	CA-CB	7.18	1.65	1.53
2	B	331	ALA	CA-CB	-6.12	1.45	1.53
1	A	8	ASP	C-N	-5.90	1.25	1.33
2	B	282	ILE	CA-CB	-5.80	1.47	1.54
2	B	329	ILE	CG1-CD1	5.77	1.74	1.51
2	B	330	ILE	CA-CB	-5.77	1.47	1.54
2	B	150	GLY	N-CA	5.72	1.51	1.45
1	A	316	ILE	CA-CB	5.43	1.61	1.54
2	B	151	ILE	CA-CB	5.20	1.60	1.54
2	B	297	ASN	N-CA	-5.10	1.40	1.46
2	B	17	VAL	CA-CB	-5.02	1.48	1.54

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60	SER	CA-C-N	13.39	139.31	120.29
2	B	60	SER	C-N-CA	13.39	139.31	120.29
1	A	162	LYS	CA-C-N	-8.81	108.55	122.73
1	A	162	LYS	C-N-CA	-8.81	108.55	122.73
2	B	62	ARG	O-C-N	-8.49	111.29	122.59
1	A	236	THR	CA-C-N	8.16	130.04	119.84
1	A	236	THR	C-N-CA	8.16	130.04	119.84
2	B	306	TYR	CA-C-N	-8.11	111.63	119.90
2	B	306	TYR	C-N-CA	-8.11	111.63	119.90
1	A	112	ASN	N-CA-C	-8.04	101.97	112.41
1	A	337	ILE	CB-CA-C	7.63	121.92	110.63
1	A	85	ILE	N-CA-C	7.16	118.60	108.93
1	A	262	GLY	CA-C-N	6.96	128.54	119.84
1	A	262	GLY	C-N-CA	6.96	128.54	119.84
1	A	336	PHE	CA-C-N	-6.91	114.09	123.14
1	A	336	PHE	C-N-CA	-6.91	114.09	123.14
2	B	212	ILE	CB-CA-C	-6.77	103.01	112.14
1	A	296	ARG	CA-C-N	-6.62	111.69	122.81
1	A	296	ARG	C-N-CA	-6.62	111.69	122.81
1	A	163	ASN	N-CA-C	6.62	120.26	112.72
2	B	101	HIS	CA-C-N	-6.44	114.15	120.52
2	B	101	HIS	C-N-CA	-6.44	114.15	120.52
1	A	285	THR	CA-C-N	-6.38	114.20	120.52
1	A	285	THR	C-N-CA	-6.38	114.20	120.52
2	B	12	ASN	N-CA-C	6.38	119.22	107.99
2	B	145	SER	N-CA-C	-6.31	104.21	112.41
1	A	222	LEU	N-CA-C	-6.28	104.13	110.97
1	A	341	ILE	CA-C-N	-6.07	117.53	121.65
1	A	341	ILE	C-N-CA	-6.07	117.53	121.65
1	A	411	LEU	N-CA-C	-6.06	100.13	109.76
2	B	235	SER	N-CA-C	6.04	119.48	111.75
2	B	69	TYR	CA-C-N	6.00	125.88	119.28
2	B	69	TYR	C-N-CA	6.00	125.88	119.28
1	A	268	ASN	CA-C-N	5.97	127.31	119.84
1	A	268	ASN	C-N-CA	5.97	127.31	119.84
1	A	333	TYR	CA-C-N	-5.96	112.35	118.85
1	A	333	TYR	C-N-CA	-5.96	112.35	118.85
1	A	37	GLU	N-CA-C	-5.95	104.88	111.36
1	A	296	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	A	326	TRP	N-CA-C	5.82	121.04	113.88
1	A	5	ARG	CG-CD-NE	-5.77	99.31	112.00
1	A	295	ARG	CA-C-N	-5.63	115.29	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	ARG	C-N-CA	-5.63	115.29	122.77
2	B	366	GLY	N-CA-C	5.56	123.68	112.34
2	B	321	ALA	CA-C-N	5.56	125.57	119.90
2	B	321	ALA	C-N-CA	5.56	125.57	119.90
2	B	289	ILE	N-CA-C	5.53	119.89	112.98
1	A	265	ASN	N-CA-C	-5.45	108.41	114.62
2	B	253	GLU	N-CA-C	-5.42	105.54	111.82
1	A	114	ILE	N-CA-C	5.37	115.58	107.75
1	A	364	SER	CA-C-N	5.35	126.53	119.84
1	A	364	SER	C-N-CA	5.35	126.53	119.84
2	B	334	GLU	CA-C-N	5.34	128.82	120.82
2	B	334	GLU	C-N-CA	5.34	128.82	120.82
1	A	64	ILE	N-CA-CB	5.33	116.68	110.65
2	B	245	GLY	N-CA-C	5.33	125.81	113.18
2	B	65	LEU	N-CA-C	5.30	117.73	109.52
1	A	335	ASN	N-CA-C	5.29	117.96	110.50
2	B	183	ARG	N-CA-C	-5.29	105.20	110.97
1	A	239	GLU	N-CA-C	-5.27	105.99	112.90
2	B	61	LYS	N-CA-C	5.27	117.10	111.36
2	B	62	ARG	CA-C-N	5.25	131.69	121.41
2	B	62	ARG	C-N-CA	5.25	131.69	121.41
1	A	160	LEU	CA-C-N	5.21	125.50	119.92
1	A	160	LEU	C-N-CA	5.21	125.50	119.92
2	B	142	LEU	N-CA-C	-5.18	105.71	112.23
1	A	384	ASN	N-CA-C	5.17	117.81	110.10
1	A	225	LYS	N-CA-C	-5.16	105.73	111.36
1	A	156	ILE	N-CA-C	5.16	115.52	107.99
1	A	49	ILE	N-CA-C	5.15	115.88	110.62
2	B	151	ILE	CA-C-N	-5.13	116.45	123.12
2	B	151	ILE	C-N-CA	-5.13	116.45	123.12
1	A	43	LYS	N-CA-C	-5.12	105.59	111.07
1	A	275	VAL	N-CA-C	5.06	115.21	110.30
2	B	163	VAL	CA-C-N	5.06	125.21	119.90
2	B	163	VAL	C-N-CA	5.06	125.21	119.90
2	B	193	LEU	N-CA-C	-5.04	105.70	111.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	ILE	Peptide
1	A	85	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3364	0	3346	174	0
2	B	2817	0	2793	149	0
3	A	43	0	25	3	0
4	B	1	0	0	0	0
5	B	31	0	12	3	0
6	B	29	0	31	5	0
7	A	41	0	0	3	0
7	B	38	0	0	2	0
All	All	6364	0	6207	318	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 25.

All (318) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HH11	1:A:296:ARG:CG	1.64	1.09
1:A:296:ARG:HH11	1:A:296:ARG:HG3	1.10	1.07
2:B:59:GLN:HB2	6:B:901:LAR:H223	1.33	1.05
2:B:209:VAL:HA	2:B:212:ILE:HD12	1.43	0.97
1:A:107:ARG:HG2	1:A:114:ILE:HG12	1.47	0.96
2:B:193:LEU:O	2:B:196:ARG:HB3	1.66	0.95
1:A:146:ASN:HA	1:A:196:GLU:OE2	1.68	0.92
2:B:314:GLN:HB2	2:B:329:ILE:HG12	1.51	0.92
1:A:132:LYS:NZ	1:A:357:ARG:HH11	1.69	0.89
2:B:88:HIS:CE1	2:B:93:GLU:HG2	2.09	0.87
1:A:240:LEU:O	1:A:243:VAL:HG12	1.73	0.87
1:A:132:LYS:HZ3	1:A:357:ARG:NH1	1.72	0.86
1:A:132:LYS:HZ3	1:A:357:ARG:HH11	0.87	0.85
1:A:146:ASN:HD22	1:A:196:GLU:HG2	1.39	0.85
2:B:267:ILE:HG23	2:B:267:ILE:O	1.78	0.82
2:B:242:LEU:CD2	2:B:248:ILE:HG23	2.09	0.82
1:A:296:ARG:HD2	1:A:349:PHE:CD1	2.16	0.81
2:B:332:PRO:O	2:B:335:ARG:HB2	1.81	0.80
1:A:86:ASP:O	1:A:87:LYS:HD3	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:SER:OG	2:B:176:MET:HE2	1.81	0.79
1:A:254:ILE:O	1:A:258:LEU:HD23	1.82	0.79
2:B:37:ARG:O	2:B:65:LEU:HB2	1.83	0.79
1:A:296:ARG:HD2	1:A:349:PHE:HD1	1.48	0.79
2:B:59:GLN:HB2	6:B:901:LAR:C22	2.11	0.79
2:B:267:ILE:O	2:B:267:ILE:CG2	2.30	0.79
1:A:185:ILE:HD12	1:A:205:ALA:HB1	1.65	0.78
2:B:5:THR:HG23	2:B:6:THR:H	1.48	0.78
1:A:100:PHE:O	1:A:101:ALA:HB3	1.82	0.77
1:A:5:ARG:NH2	1:A:88:PRO:O	2.18	0.77
1:A:274:LYS:O	1:A:278:ILE:HG13	1.85	0.76
1:A:268:ASN:O	1:A:270:GLU:N	2.19	0.75
2:B:115:ASN:HD22	2:B:115:ASN:H	1.35	0.74
1:A:346:MET:HG3	1:A:349:PHE:CZ	2.23	0.74
2:B:56:ASP:C	2:B:58:ALA:H	1.96	0.73
1:A:240:LEU:O	1:A:244:ASN:ND2	2.21	0.72
1:A:171:ASN:HD22	1:A:172:SER:H	1.35	0.72
1:A:296:ARG:CG	1:A:296:ARG:NH1	2.39	0.72
1:A:145:GLY:O	1:A:150:LYS:NZ	2.23	0.72
2:B:82:MET:O	2:B:85:ILE:HB	1.90	0.71
1:A:331:ILE:HD12	1:A:332:THR:H	1.55	0.71
2:B:232:SER:O	2:B:233:SER:HB3	1.92	0.70
2:B:98:PRO:O	2:B:129:VAL:HG12	1.92	0.69
1:A:171:ASN:O	1:A:172:SER:C	2.35	0.69
2:B:325:MET:HE3	2:B:325:MET:HA	1.72	0.69
2:B:61:LYS:O	2:B:63:GLY:N	2.26	0.68
2:B:12:ASN:HD21	2:B:86:TRP:HE1	1.41	0.68
2:B:59:GLN:CB	6:B:901:LAR:H223	2.17	0.68
1:A:247:MET:HB2	1:A:375:TYR:CE2	2.28	0.68
1:A:248:ARG:NH1	2:B:76:ILE:O	2.26	0.68
1:A:296:ARG:HG3	1:A:296:ARG:NH1	1.96	0.68
2:B:96:VAL:HB	2:B:101:HIS:CE1	2.30	0.67
2:B:274:ILE:HG23	2:B:313:MET:HE1	1.76	0.66
1:A:80:ILE:HD11	1:A:178:LEU:HG	1.77	0.66
2:B:97:ALA:O	2:B:99:GLU:N	2.29	0.66
2:B:244:ASP:O	2:B:246:GLN:NE2	2.30	0.65
1:A:132:LYS:HE2	1:A:408:ASP:HB2	1.78	0.64
1:A:99:LYS:HE3	7:A:532:HOH:O	1.99	0.63
1:A:300:GLN:HB3	3:A:500:TAD:N3A	2.14	0.63
2:B:115:ASN:HD22	2:B:115:ASN:N	1.95	0.63
2:B:156:GLY:HA3	5:B:380:ATP:O3G	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LEU:HD12	2:B:243:PRO:HD2	1.81	0.63
1:A:146:ASN:ND2	1:A:196:GLU:HG2	2.13	0.62
1:A:106:ILE:HG22	1:A:107:ARG:HG3	1.82	0.62
1:A:295:ARG:HD2	1:A:337:ILE:HD11	1.82	0.62
1:A:89:ILE:HG21	1:A:166:MET:CE	2.30	0.62
1:A:243:VAL:HG22	1:A:247:MET:SD	2.39	0.62
1:A:228:TYR:CE2	1:A:367:ALA:HA	2.35	0.62
1:A:296:ARG:NH1	7:A:531:HOH:O	2.33	0.61
2:B:131:ALA:HB1	2:B:356:TRP:HB3	1.83	0.61
2:B:78:ASN:ND2	2:B:81:ASP:OD1	2.34	0.60
1:A:26:ARG:HH11	1:A:26:ARG:HG2	1.67	0.60
2:B:102:PRO:HB3	2:B:131:ALA:HB3	1.82	0.60
1:A:300:GLN:O	1:A:302:PHE:N	2.35	0.60
2:B:242:LEU:HD21	2:B:248:ILE:CG2	2.31	0.60
1:A:341:ILE:HD11	1:A:379:TYR:HB3	1.83	0.60
2:B:88:HIS:HE1	2:B:93:GLU:HG2	1.61	0.60
1:A:106:ILE:HG22	1:A:107:ARG:CG	2.31	0.60
1:A:171:ASN:HD22	1:A:172:SER:N	1.99	0.60
2:B:56:ASP:O	2:B:58:ALA:N	2.35	0.60
2:B:157:ASP:O	2:B:183:ARG:HB2	2.01	0.59
2:B:371:HIS:O	2:B:372:ARG:NH2	2.35	0.59
1:A:126:ILE:HG22	1:A:131:PHE:CZ	2.37	0.59
2:B:242:LEU:HD21	2:B:248:ILE:HG23	1.83	0.59
1:A:346:MET:CG	1:A:349:PHE:CZ	2.84	0.59
1:A:132:LYS:HG3	1:A:408:ASP:CG	2.28	0.59
2:B:33:SER:O	2:B:70:PRO:HD2	2.03	0.59
1:A:127:GLN:H	1:A:127:GLN:HE21	1.50	0.58
2:B:61:LYS:O	2:B:62:ARG:C	2.47	0.58
2:B:54:VAL:HG12	2:B:55:GLY:N	2.18	0.58
1:A:277:ASN:O	1:A:280:ASN:N	2.37	0.57
1:A:5:ARG:HG3	1:A:6:PRO:O	2.04	0.57
1:A:107:ARG:HD3	1:A:113:GLU:O	2.04	0.57
1:A:295:ARG:HD2	1:A:337:ILE:CD1	2.35	0.57
1:A:282:LEU:HD11	1:A:382:LEU:HD23	1.86	0.57
2:B:196:ARG:O	2:B:196:ARG:HG3	2.05	0.57
1:A:126:ILE:HG13	1:A:126:ILE:O	2.05	0.57
2:B:155:SER:OG	2:B:160:THR:CG2	2.52	0.57
1:A:393:LYS:HD3	1:A:394:VAL:N	2.21	0.56
2:B:205:GLU:HA	2:B:208:ILE:HD13	1.86	0.56
2:B:37:ARG:O	2:B:65:LEU:CB	2.54	0.56
1:A:127:GLN:HE21	1:A:128:ASP:H	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:PHE:HZ	2:B:123:MET:CE	2.18	0.56
1:A:20:GLU:CD	1:A:141:LEU:HD22	2.30	0.56
2:B:250:ILE:HD11	2:B:254:ARG:HA	1.88	0.56
2:B:300:SER:HA	2:B:335:ARG:HG2	1.88	0.55
2:B:12:ASN:ND2	2:B:86:TRP:HE1	2.02	0.55
1:A:89:ILE:HD13	1:A:166:MET:HE1	1.88	0.55
1:A:255:ASN:O	1:A:259:ILE:HG12	2.06	0.55
2:B:252:ASN:ND2	2:B:256:ARG:HH21	2.04	0.55
1:A:399:ASP:C	1:A:399:ASP:OD2	2.48	0.55
1:A:130:LEU:N	1:A:130:LEU:HD12	2.22	0.55
1:A:26:ARG:HG2	1:A:26:ARG:NH1	2.20	0.55
2:B:321:ALA:HB1	2:B:322:PRO:HD2	1.89	0.55
1:A:277:ASN:N	1:A:277:ASN:HD22	2.05	0.54
1:A:345:ASN:C	1:A:346:MET:HG2	2.32	0.54
2:B:306:TYR:CZ	5:B:380:ATP:H2	2.25	0.54
1:A:274:LYS:HB3	1:A:278:ILE:HD11	1.89	0.54
1:A:231:TRP:O	1:A:235:LEU:HG	2.07	0.53
1:A:28:GLU:HG3	1:A:29:LYS:N	2.23	0.53
2:B:56:ASP:C	2:B:58:ALA:N	2.64	0.53
1:A:134:ASP:CG	1:A:357:ARG:HH12	2.17	0.53
2:B:252:ASN:HD22	2:B:253:GLU:N	2.06	0.53
2:B:352:PHE:O	2:B:355:MET:HB2	2.08	0.53
1:A:136:PHE:CE2	1:A:180:GLU:HG3	2.44	0.53
1:A:335:ASN:ND2	3:A:500:TAD:N7A	2.57	0.53
1:A:150:LYS:HE3	1:A:196:GLU:HG3	1.89	0.53
1:A:310:GLU:HA	1:A:318:ASN:OD1	2.09	0.53
2:B:358:THR:O	2:B:361:GLU:HB2	2.09	0.53
1:A:161:PRO:HD3	1:A:207:ILE:HD12	1.91	0.53
1:A:378:GLU:C	1:A:379:TYR:CD2	2.87	0.53
2:B:205:GLU:O	2:B:208:ILE:HB	2.09	0.53
1:A:100:PHE:O	1:A:101:ALA:CB	2.50	0.53
2:B:148:THR:HG23	2:B:167:GLU:HA	1.90	0.53
2:B:97:ALA:HB1	2:B:99:GLU:OE1	2.08	0.52
1:A:61:ASP:OD2	1:A:62:TYR:N	2.42	0.52
1:A:115:SER:HB2	1:A:118:LYS:HG3	1.90	0.52
1:A:194:VAL:HA	1:A:198:LYS:O	2.08	0.52
2:B:202:THR:OG1	2:B:205:GLU:N	2.43	0.52
2:B:362:TYR:O	2:B:365:ALA:O	2.28	0.52
2:B:14:SER:HB3	2:B:71:ILE:HG22	1.92	0.52
1:A:254:ILE:H	1:A:254:ILE:HD12	1.74	0.52
1:A:291:LEU:CD1	1:A:293:VAL:HG13	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:VAL:O	2:B:372:ARG:N	2.43	0.52
1:A:257:TYR:HD1	1:A:258:LEU:HD22	1.75	0.51
1:A:243:VAL:HG13	1:A:244:ASN:N	2.24	0.51
1:A:243:VAL:HG13	1:A:244:ASN:OD1	2.10	0.51
2:B:130:PRO:O	2:B:359:LYS:N	2.42	0.51
1:A:122:LEU:HD23	1:A:201:ILE:HD12	1.93	0.51
2:B:98:PRO:HB2	2:B:127:PHE:O	2.10	0.51
2:B:120:THR:O	2:B:121:GLN:C	2.52	0.51
1:A:136:PHE:CD2	1:A:180:GLU:HG3	2.46	0.51
1:A:266:ASN:N	1:A:267:PRO:HD3	2.26	0.51
1:A:246:TYR:CE2	1:A:336:PHE:HB2	2.46	0.51
2:B:217:CYS:HA	2:B:254:ARG:O	2.11	0.50
2:B:34:ILE:HD12	2:B:34:ILE:O	2.12	0.50
2:B:306:TYR:O	2:B:307:PRO:C	2.51	0.50
2:B:83:GLU:O	2:B:84:LYS:C	2.54	0.50
1:A:233:ASN:O	1:A:235:LEU:N	2.45	0.50
1:A:222:LEU:O	1:A:223:TRP:C	2.55	0.50
2:B:279:TYR:CE1	2:B:283:MET:HE3	2.45	0.50
1:A:56:ARG:NH1	1:A:70:GLU:OE2	2.45	0.50
1:A:171:ASN:ND2	1:A:172:SER:H	2.07	0.50
1:A:246:TYR:HE2	1:A:336:PHE:HB2	1.76	0.49
2:B:90:PHE:CZ	2:B:123:MET:CE	2.95	0.49
2:B:209:VAL:O	2:B:210:ARG:C	2.55	0.49
2:B:124:PHE:CE1	2:B:362:TYR:HB2	2.47	0.49
2:B:372:ARG:HA	2:B:372:ARG:NE	2.28	0.49
2:B:115:ASN:N	2:B:115:ASN:ND2	2.60	0.49
1:A:89:ILE:CD1	1:A:166:MET:HE1	2.43	0.49
1:A:106:ILE:HD11	1:A:122:LEU:HD22	1.94	0.49
1:A:235:LEU:O	1:A:235:LEU:HD12	2.13	0.49
2:B:80:ASP:O	2:B:83:GLU:HB2	2.12	0.49
2:B:242:LEU:CD2	2:B:248:ILE:CG2	2.85	0.49
2:B:21:PHE:CD1	2:B:28:ARG:NH1	2.81	0.48
2:B:73:HIS:HD2	2:B:158:GLY:O	1.96	0.48
1:A:297:SER:HB2	1:A:301:GLU:CD	2.38	0.48
1:A:5:ARG:HB3	1:A:19:TRP:CE2	2.48	0.48
1:A:248:ARG:NH2	2:B:115:ASN:HD21	2.12	0.48
1:A:262:GLY:N	1:A:263:PRO:HD2	2.28	0.48
1:A:315:LYS:HB2	1:A:318:ASN:HD22	1.77	0.48
2:B:122:ILE:O	2:B:126:THR:HB	2.12	0.48
1:A:185:ILE:HD13	1:A:185:ILE:HA	1.62	0.48
2:B:131:ALA:HA	2:B:357:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:HG3	1:A:175:VAL:HG21	1.94	0.48
2:B:257:CYS:HB3	2:B:258:PRO:CD	2.44	0.48
2:B:287:ILE:HA	2:B:290:ARG:HG3	1.95	0.48
1:A:216:ASP:CG	1:A:219:LYS:HB2	2.38	0.48
1:A:289:SER:HA	1:A:362:LYS:HD3	1.95	0.48
2:B:88:HIS:ND1	2:B:93:GLU:HG2	2.27	0.48
1:A:158:LEU:HD21	1:A:185:ILE:HD11	1.96	0.48
1:A:257:TYR:CD1	1:A:258:LEU:HD22	2.49	0.48
2:B:155:SER:OG	2:B:160:THR:HG22	2.13	0.48
1:A:243:VAL:O	1:A:247:MET:HG2	2.13	0.47
2:B:143:TYR:C	2:B:145:SER:H	2.22	0.47
1:A:334:PRO:O	1:A:385:HIS:HB2	2.13	0.47
1:A:123:LYS:O	1:A:127:GLN:HG3	2.13	0.47
2:B:189:LEU:O	2:B:193:LEU:HB2	2.14	0.47
1:A:217:VAL:HG12	1:A:342:GLY:HA3	1.97	0.47
2:B:31:PHE:CE2	2:B:93:GLU:HG3	2.50	0.47
1:A:355:ILE:HD13	1:A:355:ILE:N	2.29	0.47
2:B:272:ALA:HB1	2:B:276:GLU:HB3	1.96	0.47
1:A:408:ASP:OD2	1:A:408:ASP:C	2.57	0.46
1:A:149:GLU:HG2	1:A:151:PRO:HD3	1.98	0.46
2:B:95:ARG:HB2	2:B:95:ARG:HH21	1.80	0.46
1:A:393:LYS:HD3	1:A:394:VAL:H	1.78	0.46
2:B:92:ASN:N	2:B:92:ASN:ND2	2.63	0.46
2:B:274:ILE:HG23	2:B:313:MET:CE	2.43	0.46
1:A:126:ILE:HG22	1:A:131:PHE:HZ	1.80	0.46
1:A:295:ARG:HB3	1:A:356:LEU:HB3	1.97	0.46
2:B:202:THR:HG23	2:B:205:GLU:OE2	2.15	0.46
2:B:107:GLU:HA	7:B:935:HOH:O	2.13	0.46
1:A:303:GLY:O	1:A:304:LEU:HD23	2.16	0.46
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.77	0.46
2:B:194:THR:O	2:B:196:ARG:N	2.48	0.46
2:B:87:HIS:O	2:B:88:HIS:C	2.57	0.46
2:B:273:GLY:O	2:B:277:THR:HG23	2.16	0.45
1:A:294:TYR:CE2	1:A:357:ARG:HG3	2.51	0.45
1:A:387:SER:HA	1:A:413:ASN:HD21	1.81	0.45
2:B:252:ASN:HD22	2:B:252:ASN:C	2.23	0.45
2:B:349:LEU:O	2:B:350:SER:C	2.59	0.45
1:A:243:VAL:CG1	1:A:244:ASN:N	2.79	0.45
2:B:267:ILE:HG22	2:B:269:MET:HG3	1.98	0.45
1:A:368:TYR:OH	1:A:379:TYR:HA	2.16	0.45
2:B:242:LEU:HD22	2:B:248:ILE:HG23	1.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASP:O	1:A:87:LYS:CD	2.58	0.45
2:B:155:SER:OG	2:B:160:THR:HG21	2.16	0.45
1:A:5:ARG:NH1	1:A:86:ASP:OD2	2.50	0.45
1:A:142:TYR:N	1:A:142:TYR:CD1	2.84	0.45
1:A:353:LYS:HA	1:A:404:LYS:HD3	1.98	0.45
2:B:54:VAL:HB	2:B:88:HIS:CD2	2.52	0.45
2:B:95:ARG:CB	2:B:95:ARG:NH2	2.80	0.45
1:A:48:GLN:O	1:A:48:GLN:HG2	2.17	0.45
2:B:7:ALA:HA	2:B:102:PRO:HD2	1.99	0.45
6:B:901:LAR:O1	6:B:901:LAR:H42	2.17	0.45
1:A:243:VAL:HG13	1:A:244:ASN:CG	2.42	0.44
2:B:21:PHE:HD1	2:B:28:ARG:NH1	2.16	0.44
1:A:52:TYR:CZ	1:A:56:ARG:HG3	2.53	0.44
1:A:132:LYS:HG3	1:A:408:ASP:OD1	2.18	0.44
2:B:121:GLN:O	2:B:122:ILE:C	2.61	0.44
2:B:54:VAL:CG1	2:B:55:GLY:N	2.80	0.44
1:A:172:SER:OG	1:A:173:ASN:N	2.50	0.44
1:A:248:ARG:HH22	2:B:115:ASN:HD21	1.65	0.44
1:A:278:ILE:HG13	1:A:278:ILE:H	1.70	0.44
1:A:300:GLN:C	1:A:302:PHE:N	2.74	0.44
1:A:87:LYS:HD2	1:A:87:LYS:HA	1.65	0.44
1:A:306:LEU:HD21	2:B:265:SER:HB2	2.00	0.44
1:A:359:ASN:ND2	1:A:359:ASN:C	2.76	0.44
1:A:218:SER:O	1:A:219:LYS:C	2.60	0.44
1:A:268:ASN:C	1:A:270:GLU:H	2.25	0.44
2:B:172:PRO:O	2:B:173:HIS:C	2.61	0.44
2:B:210:ARG:HD2	2:B:214:GLU:OE1	2.17	0.44
1:A:384:ASN:OD1	1:A:385:HIS:N	2.51	0.43
2:B:97:ALA:C	2:B:99:GLU:H	2.26	0.43
2:B:97:ALA:C	2:B:99:GLU:N	2.77	0.43
2:B:119:MET:O	2:B:123:MET:HB2	2.18	0.43
1:A:295:ARG:CD	1:A:337:ILE:HD11	2.47	0.43
2:B:301:GLY:O	2:B:302:GLY:C	2.60	0.43
1:A:302:PHE:CD2	1:A:354:ILE:HD13	2.53	0.43
1:A:125:THR:O	1:A:125:THR:HG22	2.19	0.43
1:A:134:ASP:OD2	1:A:357:ARG:NH1	2.38	0.43
2:B:92:ASN:N	2:B:92:ASN:HD22	2.16	0.43
2:B:118:LYS:O	2:B:122:ILE:HG13	2.19	0.43
2:B:108:ALA:HB2	7:B:934:HOH:O	2.18	0.43
2:B:130:PRO:HA	2:B:359:LYS:HD2	2.01	0.43
2:B:302:GLY:HA3	5:B:380:ATP:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:TYR:C	2:B:145:SER:N	2.76	0.43
1:A:361:PRO:HA	7:A:516:HOH:O	2.19	0.43
2:B:210:ARG:HH11	6:B:901:LAR:H161	1.84	0.43
2:B:21:PHE:HD1	2:B:28:ARG:HH11	1.67	0.42
2:B:265:SER:C	2:B:267:ILE:N	2.77	0.42
1:A:335:ASN:OD1	1:A:335:ASN:N	2.48	0.42
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.72	0.42
1:A:235:LEU:CD1	1:A:240:LEU:HG	2.49	0.42
2:B:172:PRO:HA	2:B:175:ILE:HD12	2.01	0.42
1:A:94:PHE:CD2	1:A:151:PRO:HD2	2.54	0.42
2:B:226:GLU:HG3	2:B:255:PHE:CE2	2.54	0.42
1:A:109:GLU:HG3	1:A:110:ASN:N	2.35	0.42
1:A:300:GLN:C	1:A:302:PHE:H	2.28	0.42
1:A:158:LEU:CD2	1:A:185:ILE:HD11	2.50	0.42
2:B:152:VAL:HA	2:B:298:VAL:O	2.19	0.42
2:B:259:GLU:O	2:B:260:THR:C	2.62	0.42
2:B:39:ARG:NH2	2:B:64:ILE:C	2.78	0.42
2:B:137:GLN:HG2	2:B:339:VAL:HG11	2.02	0.42
1:A:70:GLU:O	1:A:70:GLU:HG3	2.18	0.42
1:A:236:THR:HB	1:A:237:PRO:HD2	2.01	0.42
1:A:108:THR:O	1:A:110:ASN:N	2.53	0.41
1:A:291:LEU:HD13	1:A:293:VAL:HG13	2.01	0.41
1:A:69:ARG:HE	1:A:69:ARG:HB2	1.79	0.41
1:A:127:GLN:NE2	1:A:128:ASP:H	2.17	0.41
1:A:389:PHE:CE2	1:A:411:LEU:HD13	2.55	0.41
2:B:193:LEU:HD12	2:B:193:LEU:HA	1.67	0.41
1:A:299:PRO:HD3	2:B:270:GLU:OE1	2.19	0.41
1:A:319:ILE:O	1:A:322:PHE:N	2.54	0.41
2:B:5:THR:HG23	2:B:6:THR:N	2.26	0.41
2:B:291:LYS:HG3	2:B:325:MET:HE1	2.02	0.41
2:B:303:THR:HG22	2:B:303:THR:O	2.20	0.41
1:A:261:ASN:C	1:A:261:ASN:HD22	2.27	0.41
2:B:162:ASN:ND2	2:B:277:THR:OG1	2.54	0.41
2:B:355:MET:O	2:B:356:TRP:C	2.64	0.41
1:A:194:VAL:HG23	1:A:198:LYS:O	2.21	0.41
1:A:56:ARG:HH11	1:A:70:GLU:CD	2.29	0.41
1:A:335:ASN:OD1	3:A:500:TAD:N6A	2.52	0.41
1:A:21:LYS:O	1:A:22:LYS:C	2.64	0.41
1:A:192:ARG:H	1:A:192:ARG:HG2	1.62	0.41
1:A:297:SER:HB2	1:A:301:GLU:OE1	2.21	0.41
2:B:106:THR:HB	2:B:137:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:LEU:C	2:B:180:LEU:HD12	2.45	0.41
2:B:282:ILE:O	2:B:285:CYS:HB2	2.21	0.41
1:A:73:TYR:OH	1:A:77:ARG:HD2	2.21	0.40
1:A:269:PRO:HA	1:A:272:ASP:HB2	2.02	0.40
1:A:92:TYR:OH	1:A:157:HIS:CE1	2.74	0.40
1:A:132:LYS:HD3	1:A:134:ASP:OD2	2.20	0.40
2:B:130:PRO:O	2:B:358:THR:HA	2.20	0.40
1:A:145:GLY:O	1:A:148:ASP:OD2	2.39	0.40
2:B:173:HIS:ND1	2:B:173:HIS:N	2.69	0.40
2:B:309:ILE:HG23	2:B:310:ALA:N	2.36	0.40
2:B:87:HIS:O	2:B:89:THR:N	2.55	0.40
2:B:329:ILE:HD12	2:B:329:ILE:O	2.21	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	411/413 (100%)	346 (84%)	45 (11%)	20 (5%)	1	5
2	B	356/375 (95%)	296 (83%)	41 (12%)	19 (5%)	1	4
All	All	767/788 (97%)	642 (84%)	86 (11%)	39 (5%)	1	5

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	A	104	LYS
1	A	109	GLU
1	A	172	SER
1	A	234	LYS
1	A	237	PRO

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Mol	Chain	Res	Type
1	A	249	GLY
1	A	259	ILE
1	A	261	ASN
1	A	269	PRO
2	B	62	ARG
2	B	364	GLU
2	B	371	HIS
1	A	370	SER
1	A	375	TYR
2	B	98	PRO
2	B	196	ARG
2	B	233	SER
2	B	245	GLY
2	B	266	PHE
2	B	356	TRP
1	A	106	ILE
1	A	263	PRO
1	A	276	ASN
1	A	301	GLU
1	A	312	ASP
2	B	57	GLU
2	B	120	THR
2	B	125	GLU
2	B	126	THR
1	A	260	SER
1	A	365	PRO
2	B	83	GLU
2	B	350	SER
1	A	26	ARG
2	B	60	SER
2	B	88	HIS
2	B	38	PRO
2	B	180	LEU

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	376/376 (100%)	310 (82%)	66 (18%)	2	6
2	B	306/318 (96%)	260 (85%)	46 (15%)	3	9
All	All	682/694 (98%)	570 (84%)	112 (16%)	2	7

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	28	GLU
1	A	37	GLU
1	A	39	LEU
1	A	48	GLN
1	A	57	GLN
1	A	65	GLU
1	A	69	ARG
1	A	74	LYS
1	A	80	ILE
1	A	87	LYS
1	A	109	GLU
1	A	118	LYS
1	A	121	GLU
1	A	127	GLN
1	A	132	LYS
1	A	137	LYS
1	A	141	LEU
1	A	148	ASP
1	A	154	LEU
1	A	155	LEU
1	A	158	LEU
1	A	166	MET
1	A	170	ILE
1	A	173	ASN
1	A	174	ASP
1	A	185	ILE
1	A	192	ARG
1	A	195	ILE
1	A	201	ILE
1	A	209	ASN
1	A	218	SER
1	A	219	LYS
1	A	235	LEU
1	A	236	THR

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Mol	Chain	Res	Type
1	A	240	LEU
1	A	252	THR
1	A	258	LEU
1	A	260	SER
1	A	264	LEU
1	A	265	ASN
1	A	270	GLU
1	A	273	SER
1	A	274	LYS
1	A	275	VAL
1	A	277	ASN
1	A	278	ILE
1	A	280	ASN
1	A	284	LEU
1	A	289	SER
1	A	296	ARG
1	A	307	THR
1	A	310	GLU
1	A	316	ILE
1	A	317	GLU
1	A	324	GLU
1	A	330	VAL
1	A	335	ASN
1	A	337	ILE
1	A	341	ILE
1	A	346	MET
1	A	347	SER
1	A	355	ILE
1	A	364	SER
1	A	372	ILE
1	A	378	GLU
2	B	6	THR
2	B	14	SER
2	B	34	ILE
2	B	39	ARG
2	B	66	THR
2	B	80	ASP
2	B	84	LYS
2	B	92	ASN
2	B	115	ASN
2	B	120	THR
2	B	134	VAL

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Mol	Chain	Res	Type
2	B	148	THR
2	B	169	TYR
2	B	178	LEU
2	B	180	LEU
2	B	185	LEU
2	B	191	LYS
2	B	193	LEU
2	B	201	VAL
2	B	202	THR
2	B	205	GLU
2	B	209	VAL
2	B	210	ARG
2	B	238	LYS
2	B	241	GLU
2	B	242	LEU
2	B	248	ILE
2	B	249	THR
2	B	250	ILE
2	B	252	ASN
2	B	267	ILE
2	B	274	ILE
2	B	291	LYS
2	B	315	LYS
2	B	326	LYS
2	B	329	ILE
2	B	334	GLU
2	B	346	LEU
2	B	353	GLN
2	B	354	GLN
2	B	358	THR
2	B	359	LYS
2	B	361	GLU
2	B	368	SER
2	B	370	VAL
2	B	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	51	ASN
1	A	57	GLN

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	90	ASN
1	A	127	GLN
1	A	146	ASN
1	A	157	HIS
1	A	171	ASN
1	A	209	ASN
1	A	227	ASN
1	A	256	ASN
1	A	261	ASN
1	A	268	ASN
1	A	276	ASN
1	A	277	ASN
1	A	359	ASN
1	A	392	ASN
1	A	413	ASN
2	B	12	ASN
2	B	73	HIS
2	B	78	ASN
2	B	88	HIS
2	B	92	ASN
2	B	101	HIS
2	B	115	ASN
2	B	128	ASN
2	B	162	ASN
2	B	225	ASN
2	B	246	GLN
2	B	252	ASN
2	B	353	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TAD	A	500	-	42,47,47	1.42	5 (11%)	62,72,72	2.11	18 (29%)
5	ATP	B	380	4	32,33,33	1.42	5 (15%)	48,52,52	2.03	14 (29%)
6	LAR	B	901	-	30,31,31	2.02	5 (16%)	32,43,43	2.80	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TAD	A	500	-	-	11/30/62/62	0/5/5/5
5	ATP	B	380	4	-	3/22/38/38	0/3/3/3
6	LAR	B	901	-	-	9/23/51/51	0/2/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	LAR	O2-C1	7.15	1.49	1.34
6	B	901	LAR	C20-S1	-6.08	1.65	1.77
3	A	500	TAD	C5A-C4A	5.43	1.48	1.39
5	B	380	ATP	C5-C4	4.43	1.47	1.39
3	A	500	TAD	C5A-C6A	3.27	1.50	1.41
5	B	380	ATP	C4-N9	-3.22	1.31	1.37
5	B	380	ATP	C8-N7	3.02	1.37	1.31
3	A	500	TAD	C2N-N3N	2.72	1.36	1.30
3	A	500	TAD	C8A-N7A	2.55	1.36	1.31
6	B	901	LAR	C2-C3	2.52	1.38	1.33
5	B	380	ATP	C5-C6	2.42	1.47	1.41
3	A	500	TAD	PA-O2A	-2.31	1.50	1.56
5	B	380	ATP	C5-N7	-2.15	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	LAR	O4-C17	2.15	1.44	1.40
6	B	901	LAR	C16-C17	2.05	1.55	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	901	LAR	C19-S1-C20	9.29	97.42	92.04
6	B	901	LAR	O2-C1-C2	6.38	126.00	111.20
3	A	500	TAD	C5A-C4A-N3A	-6.06	118.37	126.72
6	B	901	LAR	O3-C17-C18	5.50	111.31	104.25
3	A	500	TAD	C1D-C2N-N3N	5.41	131.78	124.48
5	B	380	ATP	C4-C5-N7	-5.03	104.83	110.58
3	A	500	TAD	N3A-C4A-N9A	4.78	135.29	127.17
5	B	380	ATP	C5-C4-N3	-4.43	120.61	126.72
3	A	500	TAD	O2A-PA-O1A	4.40	124.28	109.95
6	B	901	LAR	O2-C1-O1	-4.39	116.31	123.34
3	A	500	TAD	C1D-C2N-S1N	-4.38	115.06	120.79
5	B	380	ATP	N3-C2-N1	-4.15	122.30	128.58
3	A	500	TAD	C2A-N3A-C4A	4.03	121.68	111.83
6	B	901	LAR	O2-C15-C14	4.03	117.24	107.77
5	B	380	ATP	C4-N9-C8	3.93	109.86	105.74
6	B	901	LAR	C15-O2-C1	3.86	127.17	117.35
5	B	380	ATP	N9-C8-N7	-3.61	108.82	113.94
6	B	901	LAR	O1-C1-C2	-3.54	117.42	126.23
5	B	380	ATP	C2-N3-C4	3.51	120.40	111.83
3	A	500	TAD	O1A-PA-C3	-3.42	100.04	109.05
5	B	380	ATP	C5-N7-C8	3.42	108.82	103.45
5	B	380	ATP	C6-C5-N7	3.34	138.53	132.09
3	A	500	TAD	C4N-N3N-C2N	3.27	114.03	110.65
5	B	380	ATP	C2-N1-C6	3.14	123.89	118.73
3	A	500	TAD	N3A-C2A-N1A	-3.12	123.85	128.58
3	A	500	TAD	C4A-C5A-N7A	-3.08	107.06	110.58
5	B	380	ATP	O4'-C1'-C2'	-2.91	100.40	106.62
3	A	500	TAD	O5B-C5B-C4B	2.71	118.23	108.99
5	B	380	ATP	N3-C4-N9	2.68	131.73	127.17
3	A	500	TAD	C2B-C1B-N9A	-2.55	106.98	113.30
3	A	500	TAD	C3D-C2D-C1D	2.49	104.63	101.69
6	B	901	LAR	C21-C3-C4	2.46	119.50	115.23
3	A	500	TAD	O2N-PN-O1N	2.37	117.68	109.95
3	A	500	TAD	C5N-C4N-N3N	-2.33	112.23	115.43
3	A	500	TAD	C4A-N9A-C8A	2.28	108.13	105.74
5	B	380	ATP	O2'-C2'-C3'	2.16	118.75	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	380	ATP	O3B-PG-O1G	-2.11	99.96	111.04
5	B	380	ATP	O2B-PB-O3B	2.07	112.86	107.27
3	A	500	TAD	O6N-C6N-C4N	2.05	122.22	120.25
3	A	500	TAD	C6A-C5A-N7A	2.04	136.02	132.09

There are no chirality outliers.

All (23) torsion outliers are listed below:

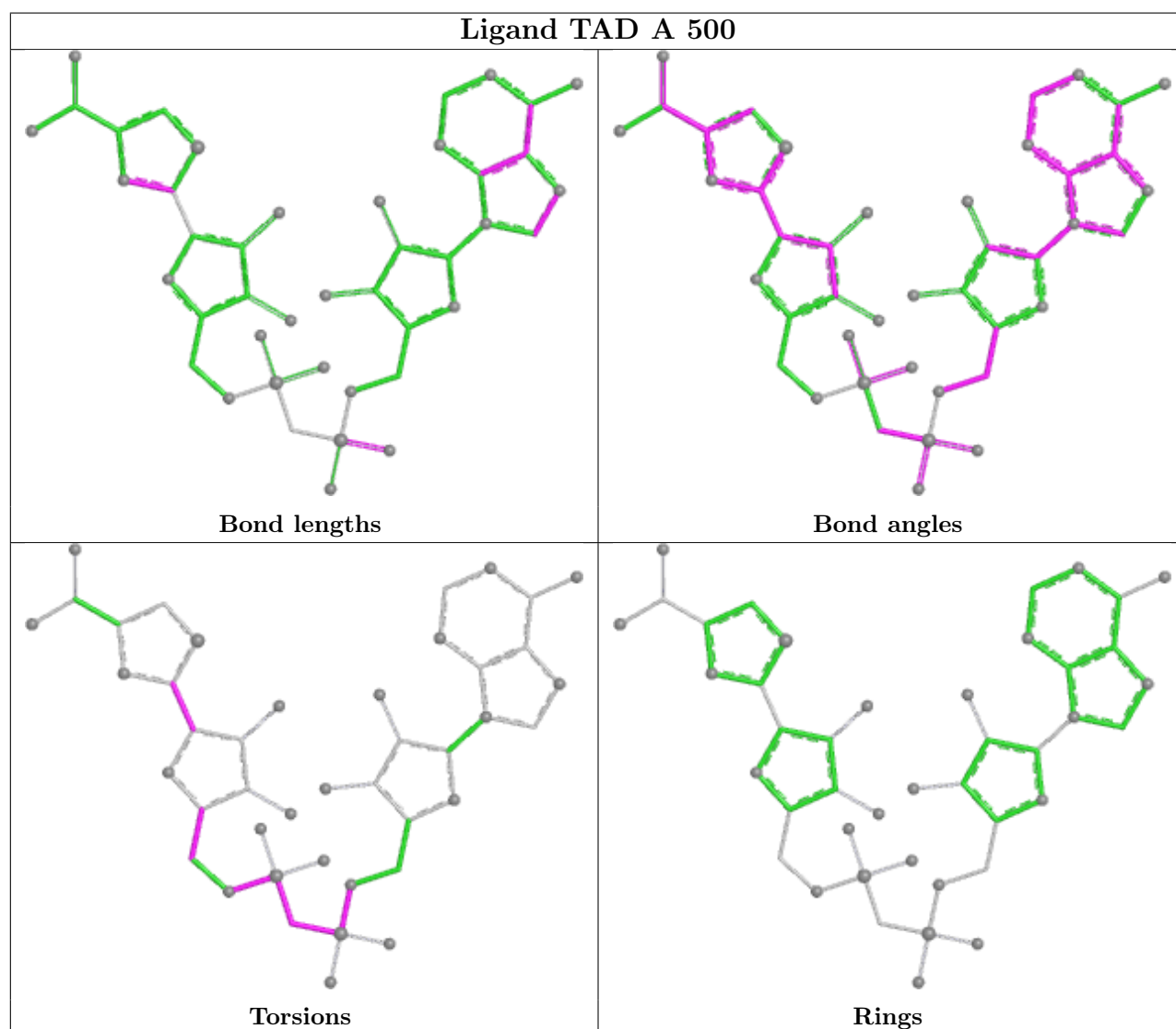
Mol	Chain	Res	Type	Atoms
3	A	500	TAD	C5B-O5B-PA-O1A
3	A	500	TAD	PN-C3-PA-O1A
3	A	500	TAD	O4D-C1D-C2N-N3N
3	A	500	TAD	O4D-C1D-C2N-S1N
5	B	380	ATP	PB-O3B-PG-O2G
5	B	380	ATP	PB-O3B-PG-O3G
6	B	901	LAR	O1-C1-O2-C15
6	B	901	LAR	C2-C1-O2-C15
6	B	901	LAR	C14-C15-O2-C1
6	B	901	LAR	O3-C17-C18-C19
6	B	901	LAR	C10-C11-C12-C13
6	B	901	LAR	C11-C12-C13-C14
6	B	901	LAR	C11-C12-C13-O3
6	B	901	LAR	C3-C4-C5-C6
3	A	500	TAD	C5D-O5D-PN-O1N
3	A	500	TAD	PN-C3-PA-O2A
3	A	500	TAD	PN-C3-PA-O5B
3	A	500	TAD	C3D-C4D-C5D-O5D
6	B	901	LAR	C4-C5-C6-C7
3	A	500	TAD	C5B-O5B-PA-O2A
3	A	500	TAD	PA-C3-PN-O1N
3	A	500	TAD	O4D-C4D-C5D-O5D
5	B	380	ATP	PB-O3B-PG-O1G

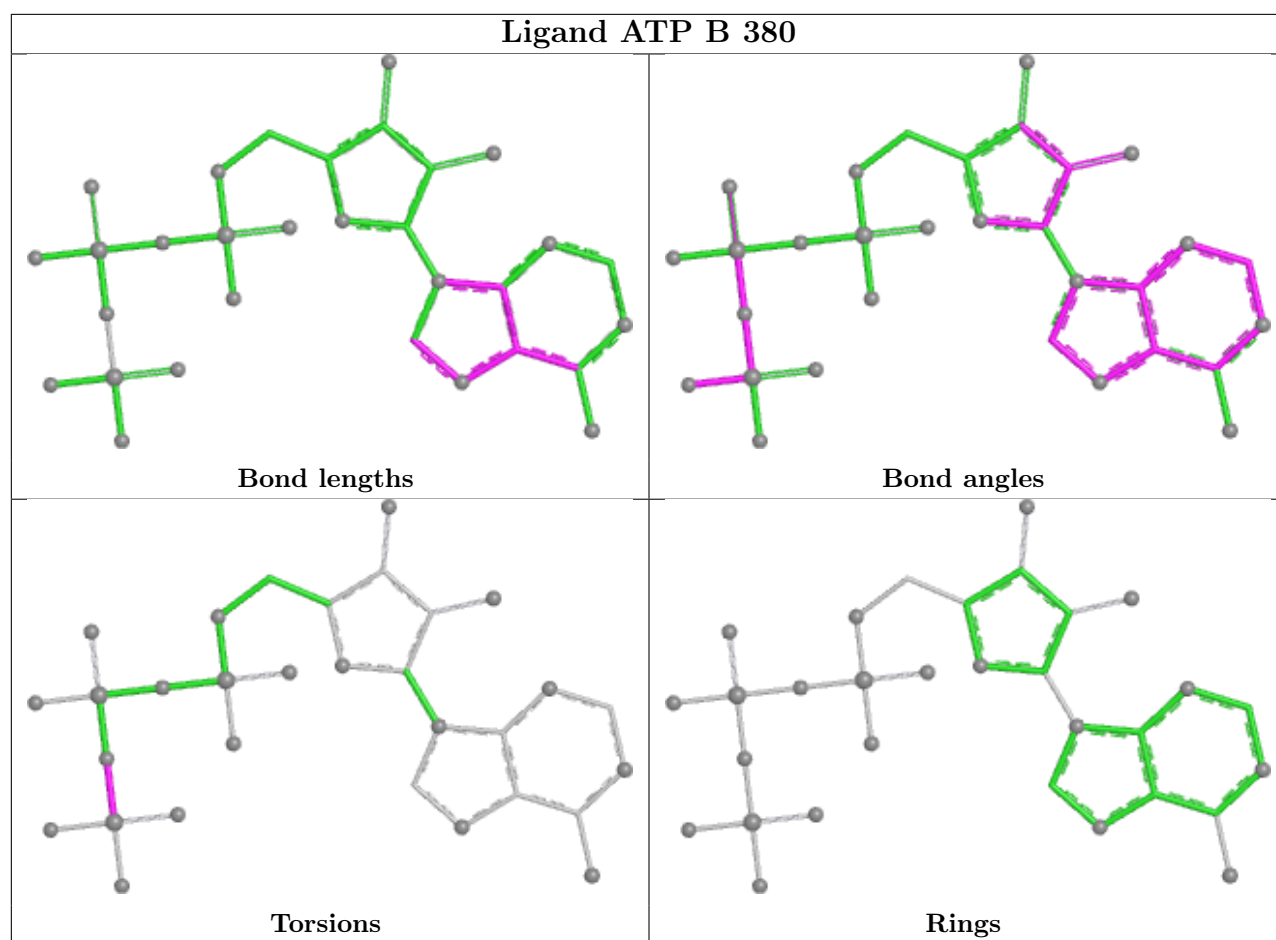
There are no ring outliers.

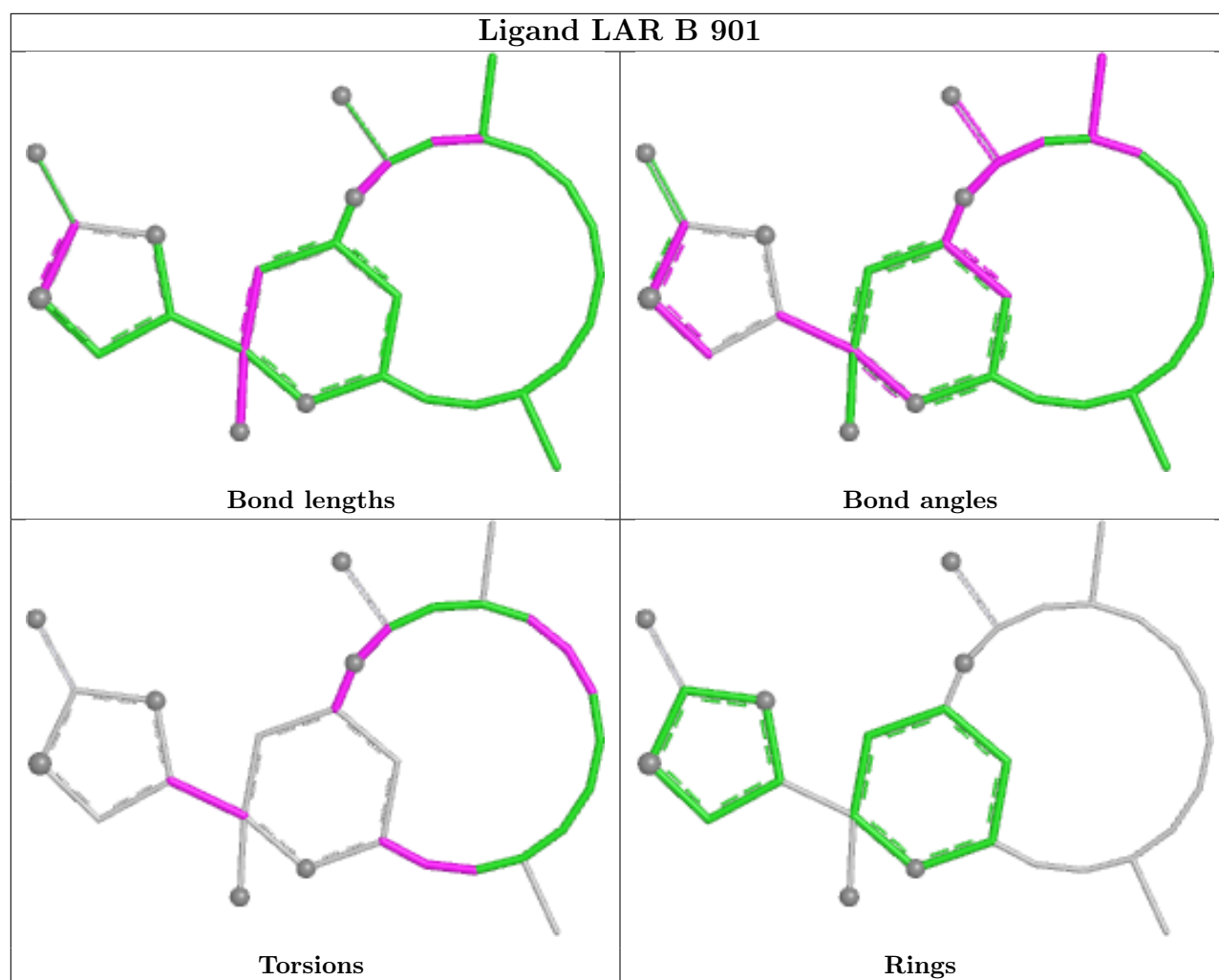
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	TAD	3	0
5	B	380	ATP	3	0
6	B	901	LAR	5	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	413/413 (100%)	0.01	18 (4%)	39	30	24, 43, 90, 108	0
2	B	360/375 (96%)	-0.02	16 (4%)	39	30	20, 46, 95, 117	0
All	All	773/788 (98%)	-0.01	34 (4%)	39	30	20, 44, 92, 117	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	TYR	4.8
2	B	374	CYS	4.1
1	A	375	TYR	3.4
1	A	271	LEU	3.2
1	A	275	VAL	3.2
2	B	79	TRP	3.1
2	B	201	VAL	3.0
1	A	249	GLY	3.0
1	A	254	ILE	3.0
2	B	55	GLY	2.9
1	A	272	ASP	2.8
2	B	329	ILE	2.8
2	B	51	ASP	2.8
2	B	5	THR	2.7
1	A	273	SER	2.7
1	A	255	ASN	2.6
2	B	66	THR	2.6
2	B	60	SER	2.5
2	B	203	THR	2.5
2	B	52	SER	2.5
1	A	374	GLY	2.5
2	B	370	VAL	2.5
1	A	413	ASN	2.5
1	A	278	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	269	PRO	2.4
1	A	248	ARG	2.4
1	A	237	PRO	2.3
2	B	202	THR	2.3
2	B	204	ALA	2.3
2	B	371	HIS	2.2
1	A	251	TYR	2.1
2	B	365	ALA	2.1
1	A	263	PRO	2.0
1	A	281	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

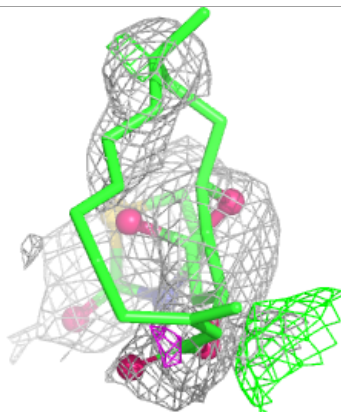
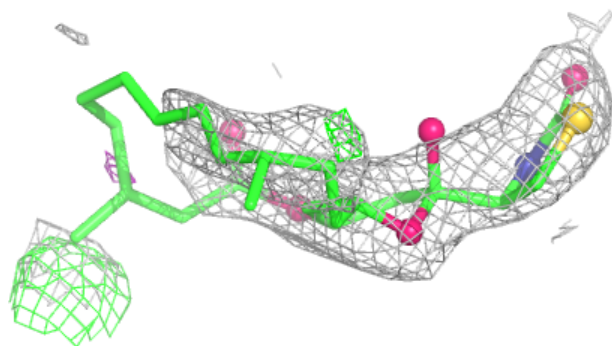
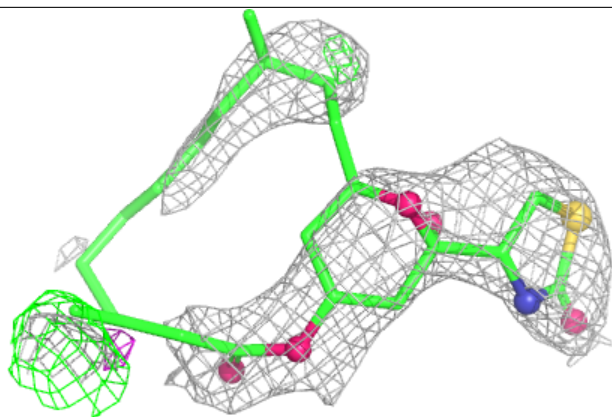
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	LAR	B	901	29/29	0.76	0.24	102,108,112,113	0
3	TAD	A	500	43/43	0.89	0.10	60,65,70,73	0
5	ATP	B	380	31/31	0.98	0.04	25,29,33,33	0
4	CA	B	500	1/1	0.99	0.04	46,46,46,46	0

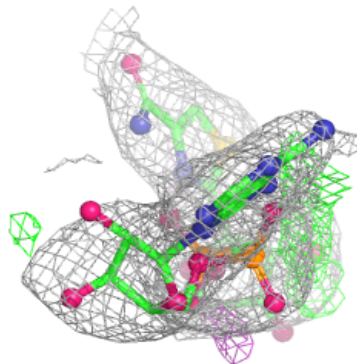
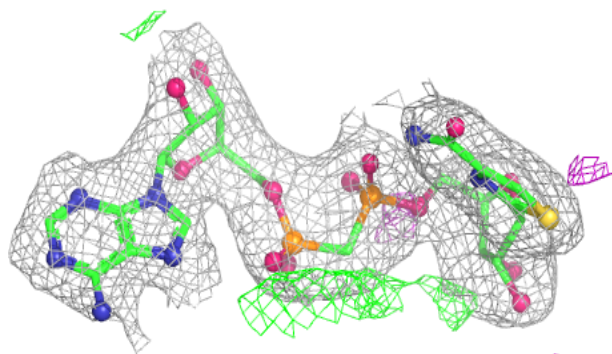
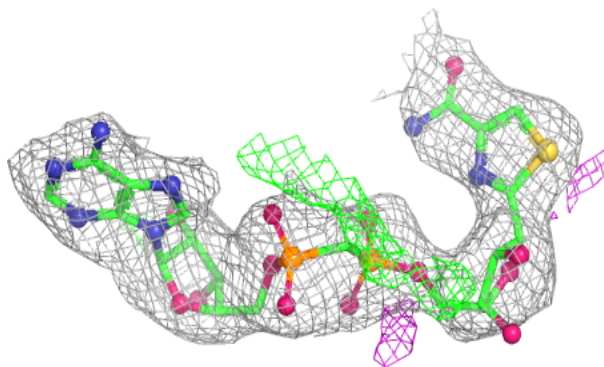
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

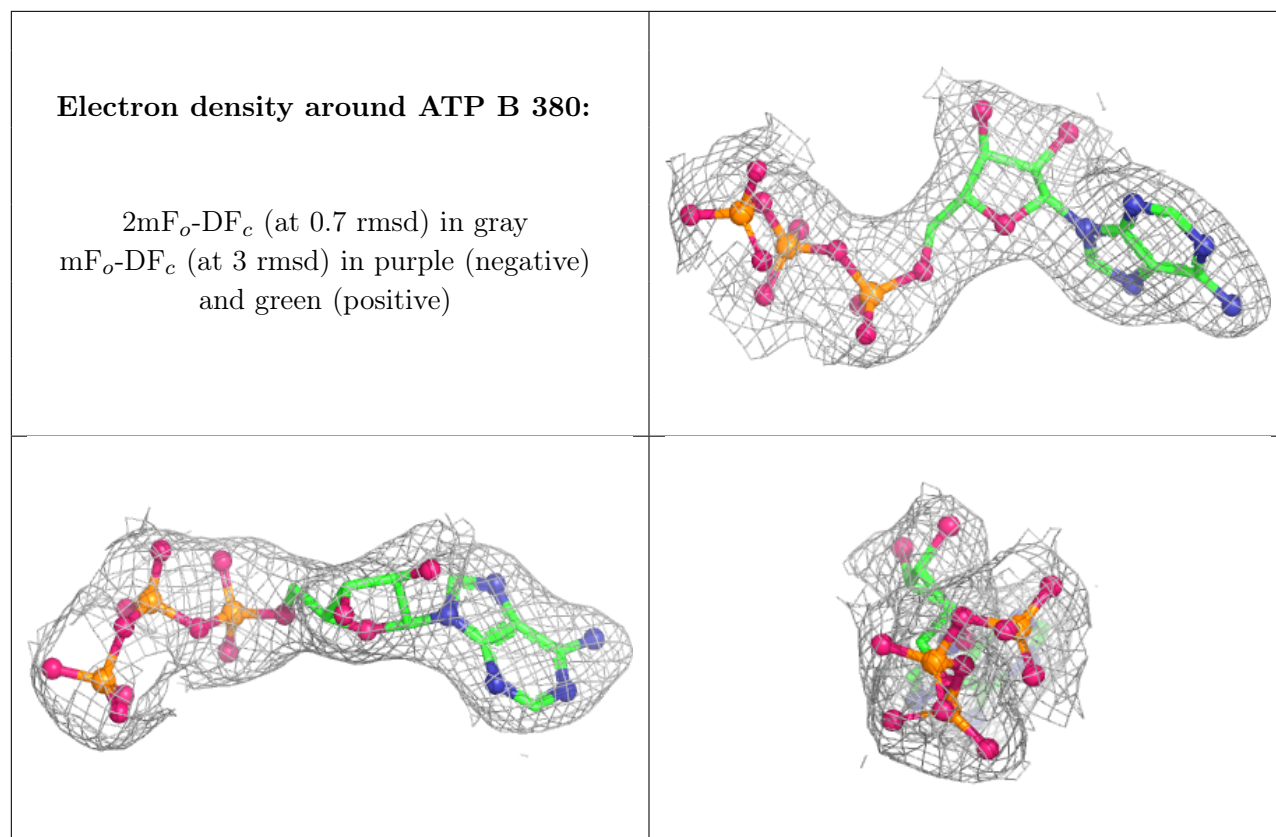
Electron density around LAR B 901:

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

**Electron density around TAD A 500:**

$2mF_o-DF_c$ (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.