



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:22 PM EDT

PDB ID : 1B76 / pdb_00001b76
Title : GLYCYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS
COMPLEXED WITH ATP
Authors : Arnez, J.G.; Moras, D.
Deposited on : 1999-01-27
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

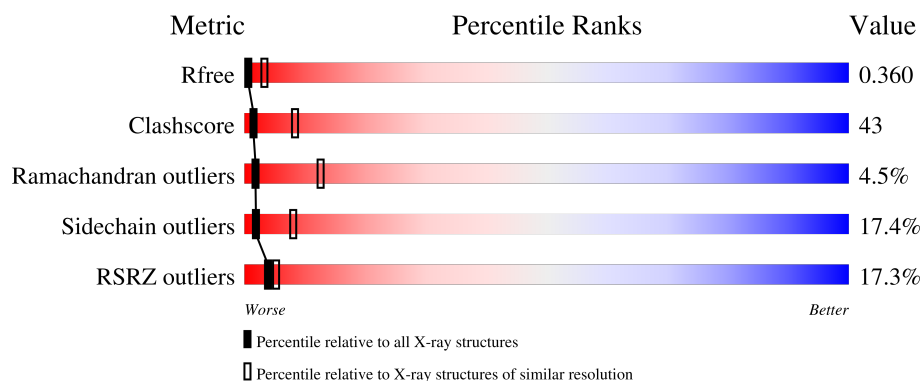
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	442	15% 34% 48% 16% •
1	B	442	20% 35% 47% 16% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8961 atoms, of which 1686 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 Glycine-tRNA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	H	N	O	S	0	0	0
			4451	2297	841	649	656	8			
1	B	442	Total	C	H	N	O	S	0	0	0
			4440	2288	839	649	656	8			

There are 44 discrepancies between the modelled and reference sequences:

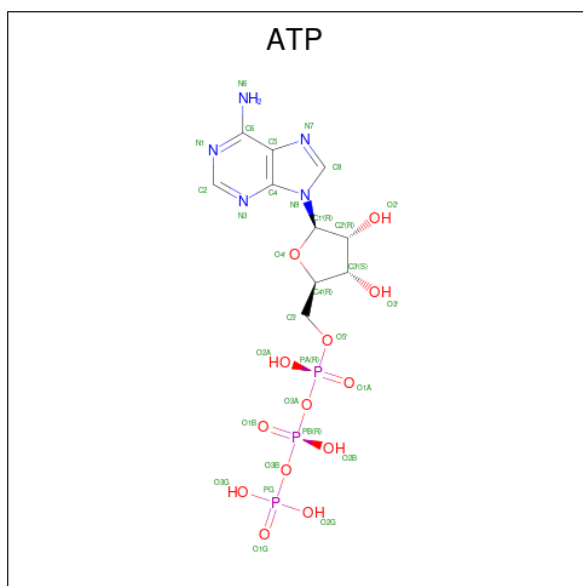
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	PRO	conflict	UNP P56206
A	91	ALA	ARG	conflict	UNP P56206
A	92	LYS	ILE	conflict	UNP P56206
A	93	ALA	THR	conflict	UNP P56206
A	94	ARG	LYS	conflict	UNP P56206
A	95	TYR	LYS	conflict	UNP P56206
A	170	GLN	LYS	conflict	UNP P56206
A	171	ASP	THR	conflict	UNP P56206
A	172	LEU	TYR	conflict	UNP P56206
A	173	ARG	VAL	conflict	UNP P56206
A	176	ARG	VAL	conflict	UNP P56206
A	177	GLY	GLU	conflict	UNP P56206
A	178	GLY	ASP	conflict	UNP P56206
A	179	ARG	GLU	conflict	UNP P56206
A	180	GLY	ALA	conflict	UNP P56206
A	181	LEU	SER	conflict	UNP P56206
A	209	GLY	PRO	conflict	UNP P56206
A	283	SER	GLU	conflict	UNP P56206
A	284	SER	LEU	conflict	UNP P56206
A	302	SER	LEU	conflict	UNP P56206
A	303	LEU	GLU	conflict	UNP P56206
A	310	GLN	ASN	conflict	UNP P56206
B	1	ALA	PRO	conflict	UNP P56206
B	91	ALA	ARG	conflict	UNP P56206
B	92	LYS	ILE	conflict	UNP P56206

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Chain	Residue	Modelled	Actual	Comment	Reference
B	93	ALA	THR	conflict	UNP P56206
B	94	ARG	LYS	conflict	UNP P56206
B	95	TYR	LYS	conflict	UNP P56206
B	170	GLN	LYS	conflict	UNP P56206
B	171	ASP	THR	conflict	UNP P56206
B	172	LEU	TYR	conflict	UNP P56206
B	173	ARG	VAL	conflict	UNP P56206
B	176	ARG	VAL	conflict	UNP P56206
B	177	GLY	GLU	conflict	UNP P56206
B	178	GLY	ASP	conflict	UNP P56206
B	179	ARG	GLU	conflict	UNP P56206
B	180	GLY	ALA	conflict	UNP P56206
B	181	LEU	SER	conflict	UNP P56206
B	209	GLY	PRO	conflict	UNP P56206
B	283	SER	GLU	conflict	UNP P56206
B	284	SER	LEU	conflict	UNP P56206
B	302	SER	LEU	conflict	UNP P56206
B	303	LEU	GLU	conflict	UNP P56206
B	310	GLN	ASN	conflict	UNP P56206

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			34	10	3	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			34	10	3	5	13	3		

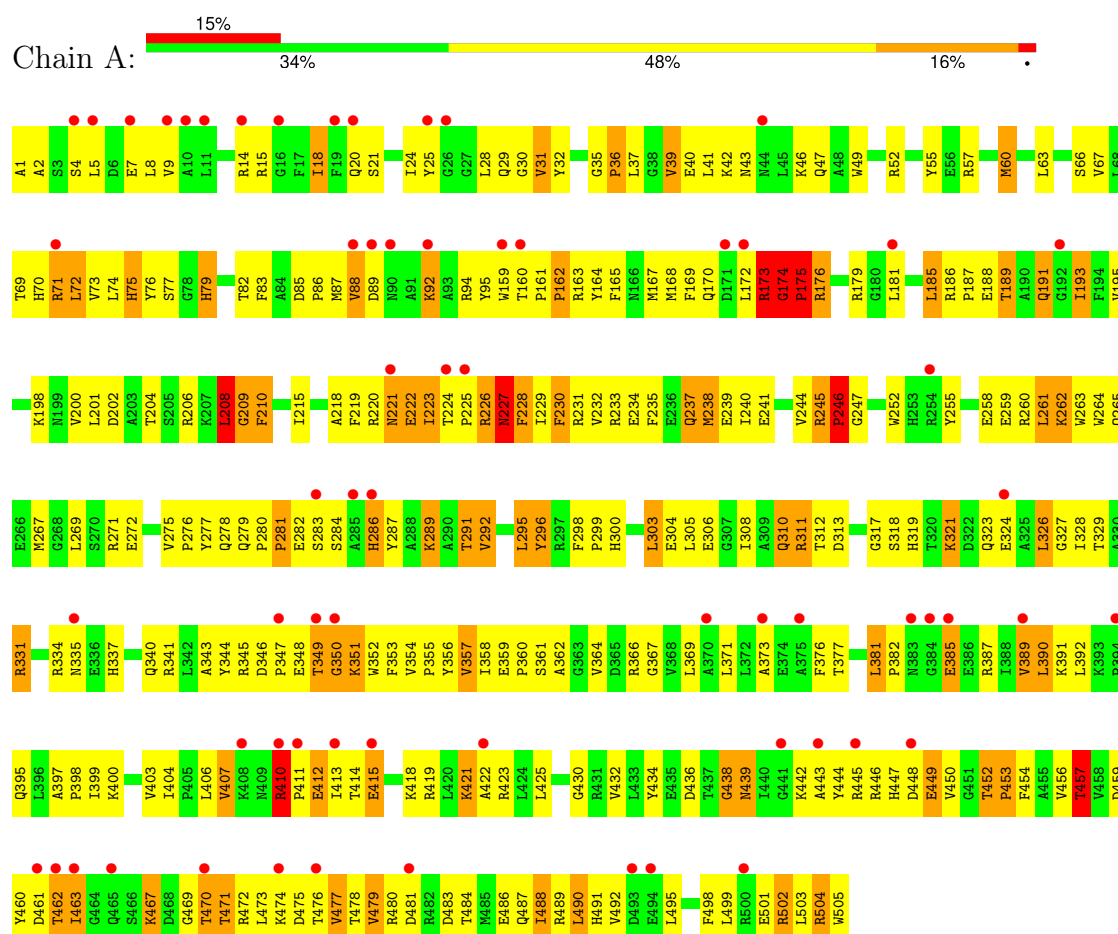
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		

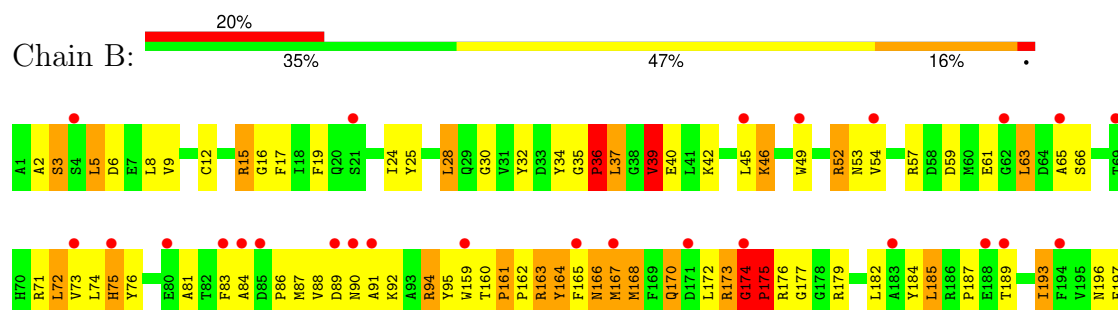
3 Residue-property plots

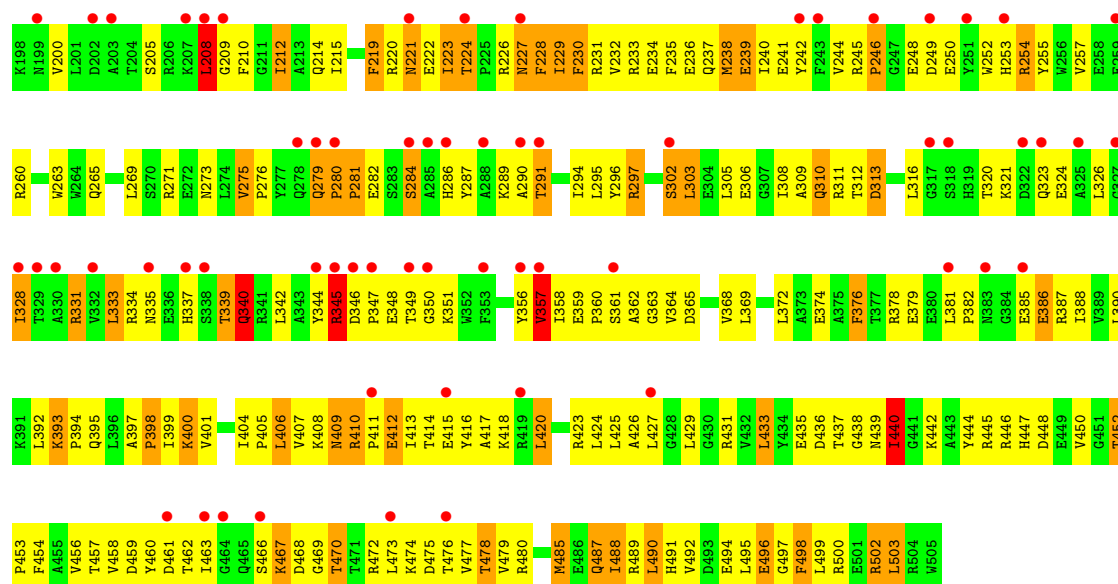
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glycine-tRNA ligase



• Molecule 1: Glycine-tRNA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.80Å 250.90Å 105.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 3.40 9.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	83.0 (9.00-3.40) 79.4 (9.00-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	9.50	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.28Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.227 , 0.318 0.298 , 0.360	Depositor DCC
R_{free} test set	784 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 94.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	8961	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: ATP

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	0.87	3/3696 (0.1%)	1.28	48/4999 (1.0%)
1	B	0.80	0/3686	1.32	43/4986 (0.9%)
All	All	0.84	3/7382 (0.0%)	1.30	91/9985 (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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	VAL	CA-CB	-7.16	1.46	1.54
1	A	403	VAL	CA-CB	-6.65	1.46	1.54
1	A	292	VAL	CA-CB	-5.13	1.48	1.54

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	LEU	N-CA-C	14.93	129.23	111.02
1	B	39	VAL	CB-CA-C	-11.08	97.96	111.81
1	B	208	LEU	N-CA-C	10.71	128.94	111.37
1	B	280	PRO	CA-C-N	9.08	131.19	119.84
1	B	280	PRO	C-N-CA	9.08	131.19	119.84
1	B	160	THR	CA-C-N	-8.92	111.19	120.38
1	B	160	THR	C-N-CA	-8.92	111.19	120.38
1	A	280	PRO	CA-C-N	8.43	130.38	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	PRO	C-N-CA	8.43	130.38	119.84
1	B	393	LYS	CA-C-N	8.32	130.24	119.84
1	B	393	LYS	C-N-CA	8.32	130.24	119.84
1	B	224	THR	CA-C-N	-8.26	111.22	119.90
1	B	224	THR	C-N-CA	-8.26	111.22	119.90
1	B	279	GLN	CA-C-N	7.81	128.43	120.38
1	B	279	GLN	C-N-CA	7.81	128.43	120.38
1	B	28	LEU	N-CA-C	-7.72	96.68	108.96
1	B	397	ALA	CA-C-N	-7.61	111.13	119.19
1	B	397	ALA	C-N-CA	-7.61	111.13	119.19
1	B	227	ASN	N-CA-C	7.45	126.67	110.80
1	A	82	THR	N-CA-C	7.38	122.38	113.23
1	B	164	TYR	N-CA-C	-7.38	101.04	110.19
1	A	289	LYS	N-CA-C	-7.29	103.26	111.14
1	B	345	ARG	N-CA-C	7.19	126.11	110.80
1	A	230	PHE	N-CA-C	7.04	118.64	110.97
1	B	54	VAL	CB-CA-C	-6.96	104.85	111.05
1	B	340	GLN	N-CA-C	6.86	119.41	110.43
1	A	176	ARG	CA-C-O	6.84	121.91	117.94
1	A	488	ILE	CB-CA-C	-6.74	101.48	110.98
1	B	452	THR	CA-C-N	6.72	128.24	119.84
1	B	452	THR	C-N-CA	6.72	128.24	119.84
1	A	381	LEU	CA-C-N	6.65	128.15	119.84
1	A	381	LEU	C-N-CA	6.65	128.15	119.84
1	A	226	ARG	N-CA-C	6.62	118.55	110.41
1	B	357	VAL	N-CA-C	6.58	117.29	108.27
1	A	247	GLY	N-CA-C	6.51	120.54	112.73
1	A	358	ILE	N-CA-C	-6.45	99.14	108.17
1	B	84	ALA	N-CA-C	-6.43	101.91	111.81
1	A	432	VAL	N-CA-C	-6.34	100.64	109.45
1	B	425	LEU	N-CA-C	-6.25	104.38	111.07
1	A	357	VAL	N-CA-C	6.23	116.81	108.27
1	A	463	ILE	CB-CA-C	-6.19	104.07	111.81
1	B	212	ILE	CB-CA-C	-6.12	101.25	111.29
1	B	75	HIS	N-CA-C	-6.09	103.39	111.24
1	B	174	GLY	C-N-CD	-6.07	100.11	125.00
1	B	3	SER	N-CA-C	5.97	118.30	111.02
1	A	448	ASP	N-CA-C	-5.96	104.13	111.40
1	B	161	PRO	CA-C-N	5.93	127.25	119.84
1	B	161	PRO	C-N-CA	5.93	127.25	119.84
1	A	228	PHE	N-CA-C	5.89	117.26	108.31
1	B	410	ARG	CA-C-N	5.87	125.74	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ARG	C-N-CA	5.87	125.74	119.28
1	A	245	ARG	CA-C-N	5.85	127.15	119.84
1	A	245	ARG	C-N-CA	5.85	127.15	119.84
1	A	503	LEU	N-CA-C	5.82	119.99	113.01
1	A	385	GLU	N-CA-C	5.79	118.45	110.35
1	B	303	LEU	N-CA-C	5.77	118.63	109.81
1	B	81	ALA	N-CA-C	5.71	117.50	111.28
1	B	248	GLU	N-CA-C	5.70	119.98	113.19
1	B	230	PHE	N-CA-C	5.65	117.12	108.30
1	A	261	LEU	N-CA-C	-5.63	105.22	111.36
1	A	191	GLN	N-CA-C	5.57	117.03	111.07
1	A	75	HIS	N-CA-C	-5.56	104.62	111.40
1	B	289	LYS	N-CA-C	-5.53	105.16	111.14
1	A	452	THR	CA-C-N	5.53	126.75	119.84
1	A	452	THR	C-N-CA	5.53	126.75	119.84
1	A	173	ARG	N-CA-C	5.52	117.72	108.23
1	A	481	ASP	N-CA-C	5.51	118.17	109.96
1	B	313	ASP	N-CA-C	-5.48	104.16	112.99
1	B	185	LEU	N-CA-C	-5.46	99.82	108.73
1	B	320	THR	N-CA-C	5.46	118.88	110.42
1	A	457	THR	N-CA-C	5.44	117.27	108.34
1	A	425	LEU	N-CA-C	-5.41	105.39	111.28
1	A	160	THR	CA-C-N	5.37	123.53	119.66
1	A	160	THR	C-N-CA	5.37	123.53	119.66
1	A	174	GLY	C-N-CD	-5.37	102.99	125.00
1	B	448	ASP	N-CA-C	-5.34	105.12	111.69
1	A	389	VAL	CB-CA-C	-5.27	103.56	110.98
1	A	185	LEU	N-CA-C	-5.23	100.64	108.96
1	A	221	ASN	N-CA-C	5.23	121.93	110.80
1	A	337	HIS	N-CA-C	5.22	120.51	114.04
1	A	227	ASN	N-CA-C	5.20	121.87	110.80
1	A	410	ARG	CA-C-N	5.15	124.94	119.28
1	A	410	ARG	C-N-CA	5.15	124.94	119.28
1	A	397	ALA	CA-C-N	-5.10	113.78	119.19
1	A	397	ALA	C-N-CA	-5.10	113.78	119.19
1	A	304	GLU	N-CA-C	5.05	117.63	110.10
1	B	503	LEU	N-CA-C	5.05	119.07	113.01
1	A	77	SER	N-CA-C	-5.03	107.15	113.28
1	A	193	ILE	N-CA-C	-5.02	106.17	110.74
1	A	208	LEU	CA-C-O	-5.01	115.55	121.07
1	A	453	PRO	N-CA-C	5.00	122.78	112.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	Sidechain

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	3610	841	3565	325	0
1	B	3601	839	3547	329	0
2	A	31	3	12	5	0
2	B	31	3	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	7275	1686	7136	626	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 43.

All (626) 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:B:88:VAL:HG22	1:B:162:PRO:HB3	1.26	1.09
1:B:413:ILE:HG12	1:B:463:ILE:HD11	1.35	1.04
1:A:366:ARG:NH1	2:A:1552:ATP:H2'	1.72	1.02
1:A:400:LYS:HD3	1:A:430:GLY:HA3	1.43	1.00
1:B:442:LYS:HA	1:B:445:ARG:HD3	1.46	0.96
1:B:331:ARG:HH11	1:B:331:ARG:HB3	1.32	0.93
1:B:245:ARG:HH22	1:B:347:PRO:HA	1.35	0.91
1:A:173:ARG:HB2	1:A:173:ARG:NH1	1.86	0.90
1:A:74:LEU:HB3	1:A:168:MET:HE1	1.52	0.89
1:A:413:ILE:CG1	1:A:463:ILE:HD11	2.04	0.88
1:A:244:VAL:HG21	1:A:252:TRP:CD1	2.09	0.86
1:A:387:ARG:HD2	1:A:445:ARG:HH22	1.41	0.84
1:A:444:TYR:CE1	1:A:480:ARG:HD3	2.12	0.83
1:A:326:LEU:HD23	1:A:341:ARG:HH21	1.44	0.83
1:B:316:LEU:HD22	1:B:342:LEU:HG	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:HIS:CD2	1:B:310:GLN:HB2	2.14	0.80
1:B:287:TYR:HD2	1:B:311:ARG:HG2	1.45	0.80
1:B:200:VAL:HG11	1:B:212:ILE:HD11	1.61	0.80
1:B:5:LEU:O	1:B:9:VAL:HG23	1.83	0.79
1:B:457:THR:HG23	1:B:478:THR:HG23	1.63	0.79
1:A:395:GLN:HB3	1:A:505:TRP:CE2	2.16	0.78
1:A:312:THR:O	1:A:356:TYR:HA	1.83	0.78
1:B:245:ARG:HH12	1:B:347:PRO:HB3	1.48	0.78
1:B:312:THR:O	1:B:356:TYR:HA	1.82	0.78
1:B:502:ARG:HD3	1:B:502:ARG:N	1.98	0.78
1:A:230:PHE:HE2	1:A:303:LEU:HD13	1.47	0.78
1:B:413:ILE:HG12	1:B:463:ILE:CD1	2.13	0.78
1:A:15:ARG:O	1:A:37:LEU:HD12	1.83	0.78
1:A:25:TYR:HD2	1:B:72:LEU:HD12	1.46	0.78
1:A:456:VAL:HG21	1:A:495:LEU:HD21	1.66	0.77
1:A:413:ILE:HG13	1:A:463:ILE:HD11	1.63	0.77
1:A:366:ARG:HH11	2:A:1552:ATP:H2'	1.51	0.76
1:A:410:ARG:HB3	1:A:412:GLU:OE1	1.86	0.74
1:A:410:ARG:NE	1:A:460:TYR:HE1	1.86	0.74
1:A:323:GLN:NE2	1:A:335:ASN:H	1.84	0.74
1:B:2:ALA:HB2	1:B:376:PHE:HB3	1.67	0.74
1:B:423:ARG:NH1	1:B:496:GLU:HG3	2.03	0.74
1:B:220:ARG:O	1:B:233:ARG:HA	1.88	0.73
1:B:364:VAL:O	1:B:368:VAL:HG23	1.89	0.73
1:A:174:GLY:H	1:B:221:ASN:HD21	1.36	0.72
1:A:173:ARG:HB2	1:A:173:ARG:HH11	1.54	0.72
1:A:277:TYR:HB3	1:A:295:LEU:HD21	1.70	0.72
1:A:323:GLN:HE22	1:A:334:ARG:HA	1.54	0.72
1:A:2:ALA:HB2	1:A:376:PHE:HB3	1.72	0.72
1:A:351:LYS:HG3	1:A:352:TRP:N	2.03	0.72
1:A:79:HIS:HA	1:A:83:PHE:HB2	1.72	0.71
1:B:461:ASP:HB2	1:B:473:LEU:HB3	1.71	0.71
1:A:88:VAL:HB	1:A:159:TRP:CZ3	2.26	0.71
1:A:244:VAL:HG21	1:A:252:TRP:NE1	2.06	0.71
1:A:413:ILE:HG12	1:A:463:ILE:HD11	1.73	0.70
1:B:287:TYR:CD2	1:B:311:ARG:HG2	2.25	0.70
1:B:15:ARG:O	1:B:37:LEU:HD23	1.92	0.70
1:A:189:THR:HG23	1:A:237:GLN:NE2	2.06	0.70
1:A:241:GLU:OE1	1:A:359:GLU:HG3	1.92	0.70
1:A:313:ASP:HB2	1:A:354:VAL:HG12	1.73	0.70
1:B:208:LEU:HG	1:B:344:TYR:CE2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HG22	1:A:224:THR:HG23	1.73	0.69
1:A:450:VAL:HG23	1:A:452:THR:HG23	1.74	0.69
1:A:28:LEU:O	1:A:31:VAL:HG13	1.92	0.69
1:A:60:MET:HE1	1:A:240:ILE:HG23	1.74	0.69
1:B:244:VAL:HG21	1:B:252:TRP:CD1	2.28	0.69
1:B:189:THR:HG22	1:B:214:GLN:OE1	1.93	0.69
1:A:404:ILE:HD13	1:A:443:ALA:HB1	1.75	0.69
1:B:87:MET:O	1:B:162:PRO:HA	1.92	0.68
1:B:165:PHE:O	1:B:167:MET:SD	2.51	0.68
1:B:331:ARG:HB3	1:B:331:ARG:NH1	2.08	0.68
1:B:208:LEU:HG	1:B:344:TYR:CD2	2.28	0.68
1:B:344:TYR:CD1	1:B:345:ARG:N	2.62	0.68
1:B:399:ILE:HD13	1:B:433:LEU:HD13	1.75	0.68
1:B:411:PRO:O	1:B:415:GLU:HG2	1.93	0.68
1:A:189:THR:HG23	1:A:237:GLN:HE21	1.59	0.68
1:B:52:ARG:HG2	1:B:263:TRP:CD1	2.28	0.68
1:A:340:GLN:HB2	1:B:24:ILE:HG22	1.75	0.68
1:A:410:ARG:O	1:A:413:ILE:HB	1.94	0.68
1:B:323:GLN:HE22	1:B:334:ARG:HA	1.57	0.68
1:A:208:LEU:O	1:A:210:PHE:N	2.27	0.67
1:B:410:ARG:HD2	1:B:412:GLU:HB2	1.76	0.67
1:B:423:ARG:HH12	1:B:496:GLU:HG3	1.59	0.67
1:B:440:ILE:HD11	1:B:444:TYR:CE2	2.29	0.67
1:A:87:MET:HE2	1:A:163:ARG:HH21	1.57	0.67
1:A:88:VAL:HA	1:A:163:ARG:NH1	2.10	0.67
1:B:406:LEU:HB2	1:B:459:ASP:HB3	1.77	0.67
1:A:480:ARG:HH11	1:A:480:ARG:HG2	1.59	0.67
1:B:265:GLN:OE1	1:B:271:ARG:HB2	1.95	0.67
1:A:5:LEU:HD23	1:A:227:ASN:HB2	1.77	0.67
1:A:267:MET:HE1	1:A:505:TRP:CZ3	2.30	0.67
1:B:244:VAL:HG11	1:B:252:TRP:HD1	1.60	0.67
1:A:287:TYR:CE2	1:A:311:ARG:CZ	2.79	0.66
1:B:454:PHE:HE1	1:B:503:LEU:HD21	1.59	0.66
1:B:345:ARG:HD3	1:B:346:ASP:N	2.10	0.66
1:B:399:ILE:CD1	1:B:433:LEU:HD13	2.26	0.66
1:A:381:LEU:HD21	1:A:387:ARG:HD3	1.77	0.66
1:A:460:TYR:HA	1:A:463:ILE:HD12	1.76	0.66
1:A:79:HIS:O	1:A:83:PHE:HB3	1.96	0.66
1:A:281:PRO:HG2	1:A:282:GLU:OE1	1.96	0.65
1:A:480:ARG:HG2	1:A:480:ARG:NH1	2.11	0.65
1:B:310:GLN:HG2	1:B:358:ILE:CD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ALA:H	1:B:214:GLN:NE2	1.95	0.65
1:B:83:PHE:CG	1:B:166:ASN:HA	2.31	0.65
1:B:323:GLN:NE2	1:B:335:ASN:H	1.95	0.65
1:B:323:GLN:NE2	1:B:334:ARG:HA	2.12	0.65
1:A:88:VAL:HB	1:A:159:TRP:HZ3	1.61	0.65
1:A:87:MET:SD	1:A:165:PHE:HB2	2.37	0.65
1:A:176:ARG:HE	1:B:163:ARG:HH12	1.45	0.65
1:A:412:GLU:CD	1:A:412:GLU:H	2.06	0.64
1:B:308:ILE:H	1:B:308:ILE:HD12	1.61	0.64
1:B:394:PRO:HB2	1:B:395:GLN:OE1	1.98	0.64
1:A:296:TYR:HD2	1:A:298:PHE:CD1	2.15	0.64
1:A:457:THR:O	1:A:477:VAL:HG12	1.98	0.64
1:A:381:LEU:HB2	1:A:385:GLU:O	1.98	0.63
1:A:25:TYR:CD2	1:B:72:LEU:HD12	2.32	0.63
1:A:461:ASP:O	1:A:474:LYS:HA	1.98	0.63
1:A:169:PHE:HE1	1:B:173:ARG:HH21	1.46	0.63
1:A:410:ARG:HD2	1:A:412:GLU:OE1	1.99	0.63
1:A:323:GLN:NE2	1:A:334:ARG:HA	2.13	0.63
1:B:414:THR:O	1:B:418:LYS:HG3	1.99	0.63
1:B:287:TYR:CE2	1:B:311:ARG:NH1	2.67	0.63
1:A:445:ARG:HA	1:A:445:ARG:NE	2.14	0.62
1:B:287:TYR:HE2	1:B:311:ARG:NH1	1.97	0.62
1:A:24:ILE:HG13	1:A:25:TYR:CD1	2.34	0.62
1:B:395:GLN:OE1	1:B:395:GLN:N	2.31	0.62
1:B:405:PRO:HD2	1:B:435:GLU:O	2.00	0.62
1:A:72:LEU:HD12	1:B:25:TYR:CG	2.34	0.62
1:A:484:THR:CB	1:A:486:GLU:HG2	2.28	0.62
1:A:246:PRO:HA	1:A:356:TYR:CD1	2.34	0.62
1:A:456:VAL:CG2	1:A:495:LEU:HD21	2.28	0.62
1:B:257:VAL:HG22	1:B:308:ILE:HB	1.82	0.62
1:B:16:GLY:HA2	1:B:19:PHE:CE1	2.35	0.61
1:A:57:ARG:HD3	1:A:60:MET:HG3	1.82	0.61
1:A:410:ARG:HG3	1:A:460:TYR:OH	2.01	0.61
1:B:2:ALA:CB	1:B:8:LEU:HD21	2.29	0.61
1:B:87:MET:HB3	1:B:94:ARG:NH2	2.15	0.61
1:A:234:GLU:OE1	1:B:66:SER:HB2	2.00	0.61
1:B:197:PHE:O	1:B:200:VAL:HG12	1.98	0.61
1:B:480:ARG:HB2	1:B:487:GLN:HG3	1.80	0.61
1:A:475:ASP:O	1:A:492:VAL:HG23	2.01	0.61
1:B:456:VAL:HG22	1:B:479:VAL:HG12	1.81	0.61
1:A:172:LEU:HB3	1:A:181:LEU:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:THR:HG23	1:A:476:THR:O	2.00	0.61
1:A:9:VAL:HG22	1:A:228:PHE:CD2	2.36	0.61
1:B:466:SER:HB2	1:B:470:THR:O	2.01	0.61
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.66	0.60
1:A:387:ARG:HB2	1:A:445:ARG:NH1	2.17	0.60
1:A:484:THR:OG1	1:A:486:GLU:HG2	2.01	0.60
1:B:450:VAL:HG23	1:B:452:THR:HG23	1.81	0.60
1:B:219:PHE:N	1:B:219:PHE:CD1	2.69	0.60
1:B:347:PRO:O	1:B:348:GLU:HG2	2.00	0.60
1:A:89:ASP:N	1:A:159:TRP:CZ3	2.70	0.60
1:A:267:MET:HE1	1:A:505:TRP:HZ3	1.66	0.60
1:A:376:PHE:CD1	1:A:376:PHE:C	2.79	0.60
1:B:229:ILE:HG23	1:B:229:ILE:O	2.01	0.60
1:A:265:GLN:HA	1:A:269:LEU:O	2.02	0.60
1:A:474:LYS:O	1:A:475:ASP:HB2	2.02	0.60
1:B:71:ARG:HE	1:B:182:LEU:HD23	1.66	0.60
1:B:2:ALA:HB3	1:B:8:LEU:HD21	1.83	0.60
1:A:407:VAL:HG21	1:A:460:TYR:CE2	2.37	0.60
1:A:348:GLU:HG3	1:A:349:THR:HG23	1.84	0.59
1:B:460:TYR:HA	1:B:463:ILE:HD12	1.84	0.59
1:A:418:LYS:O	1:A:421:LYS:HE2	2.01	0.59
1:A:484:THR:HB	1:A:486:GLU:HG2	1.84	0.59
1:B:208:LEU:O	1:B:210:PHE:N	2.35	0.59
1:A:410:ARG:NE	1:A:460:TYR:CE1	2.69	0.59
1:B:36:PRO:O	1:B:39:VAL:HG23	2.02	0.59
1:B:57:ARG:HH21	1:B:242:TYR:HE1	1.50	0.59
1:B:363:GLY:HA3	2:B:2552:ATP:H1'	1.85	0.59
1:A:4:SER:OG	1:A:7:GLU:HG3	2.02	0.59
1:A:223:ILE:CD1	1:B:175:PRO:HD3	2.33	0.59
1:B:427:LEU:CD2	1:B:496:GLU:HG2	2.32	0.59
1:A:351:LYS:HG3	1:A:352:TRP:O	2.02	0.59
2:A:1552:ATP:O1B	2:A:1552:ATP:H3'	2.03	0.59
1:A:24:ILE:HG22	1:B:340:GLN:NE2	2.18	0.58
1:A:69:THR:HB	1:A:74:LEU:HD11	1.85	0.58
1:B:168:MET:HE2	1:B:184:TYR:CD2	2.37	0.58
1:B:237:GLN:HA	1:B:364:VAL:HG23	1.84	0.58
1:B:265:GLN:HA	1:B:269:LEU:O	2.03	0.58
1:A:175:PRO:HD3	1:B:223:ILE:HD13	1.85	0.58
1:B:245:ARG:HH12	1:B:347:PRO:CB	2.16	0.58
1:A:208:LEU:HD11	1:A:355:PRO:HB3	1.84	0.58
1:B:242:TYR:HD2	1:B:244:VAL:HG23	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ARG:O	1:A:331:ARG:HG2	2.03	0.58
1:B:219:PHE:N	1:B:219:PHE:HD1	2.01	0.58
1:B:347:PRO:HG3	1:B:351:LYS:HB3	1.86	0.58
1:B:410:ARG:HG3	1:B:413:ILE:HG13	1.84	0.58
1:A:447:HIS:HA	1:A:450:VAL:HG22	1.86	0.58
1:A:504:ARG:HB3	1:A:504:ARG:NH1	2.18	0.58
1:B:260:ARG:HD3	1:B:306:GLU:OE2	2.04	0.57
1:A:230:PHE:CZ	1:A:303:LEU:HB3	2.40	0.57
1:B:253:HIS:HE1	1:B:308:ILE:O	1.86	0.57
1:B:72:LEU:O	1:B:75:HIS:HB3	2.04	0.57
1:B:333:LEU:H	1:B:333:LEU:CD2	2.17	0.57
1:B:495:LEU:O	1:B:499:LEU:HG	2.04	0.57
1:B:446:ARG:O	1:B:450:VAL:HG22	2.05	0.57
1:B:252:TRP:CZ3	1:B:255:TYR:CD2	2.93	0.57
1:A:204:THR:OG1	1:A:206:ARG:HG2	2.04	0.57
1:A:462:THR:HG21	1:A:477:VAL:HG13	1.87	0.57
1:A:221:ASN:HD21	1:B:174:GLY:HA3	1.68	0.57
1:B:46:LYS:HE3	1:B:236:GLU:OE2	2.04	0.57
1:B:252:TRP:HZ3	1:B:255:TYR:CD2	2.23	0.57
1:B:424:LEU:HA	1:B:427:LEU:HG	1.87	0.57
1:A:42:LYS:O	1:A:46:LYS:HG3	2.05	0.56
1:A:76:TYR:O	1:A:318:SER:HB3	2.04	0.56
1:B:74:LEU:HD13	1:B:168:MET:HE3	1.86	0.56
1:B:473:LEU:CD2	1:B:489:ARG:HD3	2.35	0.56
1:A:279:GLN:HG3	1:A:291:THR:HG23	1.87	0.56
1:A:287:TYR:HE2	1:A:311:ARG:CZ	2.18	0.56
1:B:86:PRO:HG3	1:B:164:TYR:HE1	1.69	0.56
1:A:319:HIS:HA	1:A:335:ASN:HD21	1.71	0.56
1:B:46:LYS:HG2	1:B:215:ILE:HG21	1.88	0.56
1:B:173:ARG:N	1:B:173:ARG:NH1	2.53	0.56
1:A:71:ARG:HE	1:A:179:ARG:HE	1.52	0.56
1:B:71:ARG:HH21	1:B:179:ARG:HE	1.53	0.56
1:B:321:LYS:HD3	1:B:339:THR:O	2.06	0.56
1:B:454:PHE:CE2	1:B:498:PHE:HE1	2.23	0.56
1:A:480:ARG:HD2	1:A:487:GLN:HE21	1.70	0.56
1:B:390:LEU:HD13	1:B:392:LEU:HD11	1.88	0.56
1:B:349:THR:OG1	1:B:350:GLY:N	2.39	0.55
1:B:475:ASP:O	1:B:492:VAL:HG23	2.06	0.55
1:A:245:ARG:HG2	1:A:246:PRO:HD2	1.88	0.55
1:B:297:ARG:CZ	1:B:302:SER:HB2	2.37	0.55
1:B:378:ARG:HH21	1:B:388:ILE:HD11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PHE:CE1	1:A:366:ARG:CZ	2.89	0.55
1:A:165:PHE:HZ	1:A:221:ASN:HD22	1.54	0.55
1:B:200:VAL:HG11	1:B:212:ILE:CD1	2.34	0.55
1:A:1:ALA:N	1:A:377:THR:HG22	2.22	0.55
1:A:504:ARG:HB3	1:A:504:ARG:HH11	1.72	0.55
1:B:52:ARG:HH11	1:B:52:ARG:CG	2.19	0.55
1:B:94:ARG:O	1:B:95:TYR:CB	2.55	0.55
1:B:345:ARG:O	1:B:347:PRO:HD3	2.06	0.55
1:A:87:MET:SD	1:A:165:PHE:CB	2.95	0.55
1:A:240:ILE:HB	1:A:360:PRO:HD2	1.87	0.55
1:B:472:ARG:HD2	1:B:472:ARG:O	2.07	0.55
1:A:390:LEU:HG	1:A:449:GLU:O	2.06	0.54
1:A:444:TYR:CD1	1:A:480:ARG:HD3	2.42	0.54
1:B:294:ILE:HD11	1:B:308:ILE:HD11	1.90	0.54
1:A:201:LEU:HD12	1:A:206:ARG:HB2	1.90	0.54
1:B:32:TYR:HB2	1:B:229:ILE:HD13	1.88	0.54
1:B:57:ARG:NH2	1:B:242:TYR:HE1	2.05	0.54
1:B:409:ASN:CG	1:B:410:ARG:N	2.65	0.54
1:A:215:ILE:HA	1:A:238:MET:HA	1.89	0.54
1:A:230:PHE:CE1	1:A:366:ARG:NE	2.76	0.54
1:A:262:LYS:HB2	1:A:262:LYS:NZ	2.23	0.54
1:A:460:TYR:HA	1:A:463:ILE:CD1	2.38	0.54
1:A:476:THR:OG1	1:A:489:ARG:NH1	2.37	0.54
1:A:413:ILE:HG22	1:A:414:THR:N	2.23	0.54
1:A:221:ASN:HD21	1:B:174:GLY:CA	2.21	0.54
1:A:295:LEU:N	1:A:295:LEU:HD22	2.23	0.54
1:B:497:GLY:O	1:B:500:ARG:HB2	2.07	0.54
1:A:72:LEU:O	1:A:75:HIS:HB3	2.08	0.53
1:B:189:THR:HB	1:B:239:GLU:OE1	2.07	0.53
1:A:490:LEU:CD1	1:A:495:LEU:HD13	2.38	0.53
1:A:296:TYR:HD2	1:A:298:PHE:CE1	2.26	0.53
1:A:344:TYR:HD2	1:A:353:PHE:CE1	2.26	0.53
1:B:86:PRO:O	1:B:87:MET:SD	2.67	0.53
1:B:173:ARG:HA	1:B:173:ARG:CZ	2.39	0.53
1:B:228:PHE:O	1:B:230:PHE:N	2.40	0.53
1:A:470:THR:HG22	1:A:471:THR:N	2.23	0.53
1:A:490:LEU:HD11	1:A:495:LEU:HD13	1.91	0.53
1:A:287:TYR:O	1:A:311:ARG:HA	2.09	0.53
1:A:277:TYR:CB	1:A:295:LEU:HD21	2.38	0.53
1:B:333:LEU:H	1:B:333:LEU:HD23	1.73	0.53
1:B:410:ARG:CD	1:B:412:GLU:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:THR:HG22	1:B:489:ARG:HG3	1.90	0.53
1:B:406:LEU:CB	1:B:459:ASP:HB3	2.39	0.53
1:A:387:ARG:HB2	1:A:445:ARG:CZ	2.39	0.52
1:B:394:PRO:O	1:B:400:LYS:HD2	2.08	0.52
1:B:226:ARG:HG3	1:B:231:ARG:HH21	1.73	0.52
1:B:381:LEU:HD21	1:B:387:ARG:HG2	1.92	0.52
1:A:15:ARG:NH2	1:A:449:GLU:HG3	2.24	0.52
1:B:310:GLN:HG2	1:B:358:ILE:HD12	1.90	0.52
1:B:427:LEU:HD13	1:B:429:LEU:HD12	1.90	0.52
1:A:220:ARG:O	1:A:233:ARG:HA	2.08	0.52
1:B:427:LEU:HD22	1:B:496:GLU:HG2	1.92	0.52
1:B:173:ARG:CZ	1:B:173:ARG:CA	2.88	0.52
1:A:279:GLN:HG2	1:A:291:THR:O	2.10	0.52
1:A:366:ARG:CZ	2:A:1552:ATP:H2'	2.37	0.52
1:B:63:LEU:HD21	1:B:196:ASN:HD22	1.74	0.52
1:B:89:ASP:HB2	1:B:94:ARG:HH21	1.75	0.52
1:A:74:LEU:CB	1:A:168:MET:HE1	2.31	0.51
1:B:89:ASP:HB2	1:B:94:ARG:NH2	2.25	0.51
1:B:376:PHE:CD1	1:B:376:PHE:C	2.88	0.51
1:B:287:TYR:CE2	1:B:311:ARG:CZ	2.93	0.51
1:A:28:LEU:HD23	1:A:31:VAL:HG11	1.92	0.51
1:A:170:GLN:N	1:A:170:GLN:OE1	2.44	0.51
1:B:57:ARG:NH2	1:B:242:TYR:CE1	2.78	0.51
1:B:215:ILE:HA	1:B:238:MET:HA	1.93	0.51
1:B:249:ASP:OD1	1:B:310:GLN:NE2	2.43	0.51
1:A:89:ASP:N	1:A:159:TRP:HZ3	2.07	0.51
1:A:173:ARG:HB2	1:A:173:ARG:CZ	2.40	0.51
1:A:340:GLN:HB2	1:B:24:ILE:CG2	2.41	0.51
1:B:87:MET:C	1:B:162:PRO:HA	2.35	0.51
1:B:230:PHE:O	2:B:2552:ATP:C2	2.64	0.51
1:A:76:TYR:CE1	1:A:335:ASN:HA	2.46	0.51
1:A:230:PHE:CD1	1:A:366:ARG:NE	2.79	0.51
1:A:313:ASP:HB2	1:A:354:VAL:CG1	2.40	0.51
1:A:491:HIS:CD2	1:A:492:VAL:N	2.78	0.51
1:A:67:VAL:HA	1:A:186:ARG:HG2	1.92	0.51
1:A:174:GLY:N	1:B:221:ASN:HD21	2.05	0.51
1:B:76:TYR:CE1	1:B:335:ASN:HA	2.46	0.51
1:A:8:LEU:HD11	1:A:373:ALA:HA	1.91	0.51
1:B:296:TYR:OH	1:B:374:GLU:HB2	2.11	0.51
1:B:220:ARG:HD3	1:B:222:GLU:OE2	2.11	0.50
1:A:230:PHE:HE1	1:A:366:ARG:CZ	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:HD11	1:A:367:GLY:HA2	1.93	0.50
1:B:404:ILE:N	1:B:404:ILE:HD12	2.27	0.50
1:A:1:ALA:H2	1:A:377:THR:HG22	1.76	0.50
1:A:376:PHE:C	1:A:376:PHE:HD1	2.18	0.50
1:A:5:LEU:CD2	1:A:227:ASN:HB2	2.40	0.50
1:A:173:ARG:CZ	1:A:173:ARG:CB	2.89	0.50
1:A:287:TYR:HD2	1:A:311:ARG:NE	2.09	0.50
1:A:24:ILE:HA	1:B:339:THR:OG1	2.12	0.50
1:B:417:ALA:HB2	1:B:458:VAL:HG21	1.93	0.50
1:B:492:VAL:O	1:B:495:LEU:HB3	2.12	0.50
1:A:87:MET:HE3	1:A:94:ARG:HB3	1.93	0.50
1:B:244:VAL:HG11	1:B:252:TRP:CD1	2.44	0.50
1:B:310:GLN:HG2	1:B:358:ILE:HD11	1.92	0.50
1:B:491:HIS:O	1:B:494:GLU:HB2	2.12	0.50
1:A:395:GLN:HB3	1:A:505:TRP:NE1	2.26	0.50
1:B:61:GLU:O	1:B:212:ILE:HA	2.12	0.50
1:B:321:LYS:HB2	1:B:339:THR:O	2.11	0.50
1:A:5:LEU:O	1:A:9:VAL:HG23	2.12	0.49
1:A:35:GLY:O	1:A:39:VAL:HG23	2.12	0.49
1:A:225:PRO:HA	1:A:231:ARG:HG2	1.94	0.49
1:B:71:ARG:NE	1:B:182:LEU:HD23	2.27	0.49
1:A:43:ASN:O	1:A:47:GLN:HG3	2.12	0.49
1:B:410:ARG:HD2	1:B:412:GLU:OE1	2.13	0.49
1:B:498:PHE:CD1	1:B:498:PHE:C	2.90	0.49
1:A:245:ARG:CG	1:A:246:PRO:HD2	2.42	0.49
1:B:420:LEU:O	1:B:424:LEU:HG	2.13	0.49
1:A:208:LEU:HG	1:A:344:TYR:CD2	2.48	0.49
1:A:279:GLN:HB2	1:A:283:SER:OG	2.12	0.49
1:A:88:VAL:CB	1:A:159:TRP:HZ3	2.24	0.49
1:B:287:TYR:O	1:B:311:ARG:HA	2.12	0.49
1:B:291:THR:HB	1:B:309:ALA:HA	1.94	0.49
1:A:215:ILE:HG12	1:A:238:MET:HB3	1.95	0.49
1:B:331:ARG:HH11	1:B:331:ARG:CB	2.14	0.49
1:B:427:LEU:HD21	1:B:496:GLU:HG2	1.94	0.49
1:A:165:PHE:HZ	1:A:221:ASN:ND2	2.11	0.49
1:B:189:THR:HG21	1:B:214:GLN:HG2	1.95	0.49
1:A:60:MET:HE1	1:A:240:ILE:CG2	2.41	0.49
1:B:416:TYR:CE2	1:B:462:THR:HG22	2.47	0.49
1:A:287:TYR:CD2	1:A:311:ARG:CZ	2.96	0.49
1:A:391:LYS:HG2	1:A:483:ASP:OD1	2.12	0.49
1:A:421:LYS:HE3	1:A:422:ALA:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ARG:NH2	1:B:388:ILE:HD11	2.28	0.49
1:B:472:ARG:HD2	1:B:472:ARG:C	2.38	0.49
1:A:187:PRO:HA	1:A:219:PHE:O	2.12	0.49
1:B:2:ALA:HB2	1:B:376:PHE:CB	2.39	0.49
1:A:406:LEU:HD23	1:A:459:ASP:HB2	1.94	0.48
1:B:454:PHE:CE1	1:B:503:LEU:HD21	2.45	0.48
1:A:28:LEU:HB3	1:A:31:VAL:CG1	2.42	0.48
1:A:287:TYR:CD2	1:A:311:ARG:NE	2.81	0.48
1:B:473:LEU:HD22	1:B:489:ARG:HH11	1.78	0.48
1:A:73:VAL:HA	1:B:25:TYR:HE2	1.78	0.48
1:A:88:VAL:C	1:A:159:TRP:HZ3	2.21	0.48
1:B:46:LYS:HE3	1:B:236:GLU:CD	2.38	0.48
1:B:87:MET:HB3	1:B:94:ARG:HH22	1.77	0.48
1:B:454:PHE:CE2	1:B:498:PHE:CE1	3.01	0.48
1:B:476:THR:HB	1:B:489:ARG:HH11	1.78	0.48
1:A:326:LEU:HD22	1:A:343:ALA:HB2	1.95	0.48
1:B:235:PHE:HB2	1:B:365:ASP:OD2	2.14	0.48
1:B:381:LEU:HB3	1:B:382:PRO:HD2	1.96	0.48
1:A:36:PRO:HB3	1:B:61:GLU:HG3	1.94	0.48
1:B:273:ASN:HB3	1:B:296:TYR:CE1	2.49	0.48
1:B:407:VAL:HG12	1:B:409:ASN:H	1.79	0.48
1:A:25:TYR:CE2	1:B:76:TYR:CD2	3.02	0.48
1:A:279:GLN:CG	1:A:291:THR:HG23	2.43	0.48
1:B:2:ALA:HB2	1:B:376:PHE:CG	2.48	0.48
1:A:467:LYS:C	1:A:469:GLY:H	2.22	0.48
1:A:92:LYS:HD2	1:A:95:TYR:CE2	2.48	0.47
1:A:24:ILE:HG13	1:A:25:TYR:HD1	1.76	0.47
1:A:319:HIS:HA	1:A:335:ASN:ND2	2.28	0.47
1:A:418:LYS:HG3	1:A:434:TYR:CE2	2.48	0.47
1:A:18:ILE:HG21	1:A:229:ILE:HD11	1.95	0.47
1:B:260:ARG:HD3	1:B:306:GLU:CD	2.39	0.47
1:B:435:GLU:OE2	1:B:447:HIS:NE2	2.47	0.47
1:B:444:TYR:CE1	1:B:480:ARG:HD3	2.49	0.47
1:B:498:PHE:C	1:B:498:PHE:HD1	2.22	0.47
1:A:246:PRO:HD3	1:A:353:PHE:CE2	2.50	0.47
1:B:254:ARG:HG3	1:B:255:TYR:N	2.30	0.47
1:B:376:PHE:C	1:B:376:PHE:HD1	2.22	0.47
1:B:405:PRO:HA	1:B:458:VAL:CG2	2.44	0.47
1:B:410:ARG:HD3	1:B:411:PRO:HD2	1.95	0.47
1:B:410:ARG:HA	1:B:411:PRO:HD3	1.78	0.47
1:B:467:LYS:C	1:B:469:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD12	1:B:35:GLY:HA2	1.97	0.47
1:A:223:ILE:HD11	1:B:175:PRO:HD3	1.97	0.47
1:A:323:GLN:HB3	1:A:328:ILE:HD12	1.95	0.47
1:A:400:LYS:HD3	1:A:430:GLY:CA	2.30	0.47
1:A:479:VAL:CG1	1:A:490:LEU:HD11	2.44	0.47
1:B:90:ASN:HB2	1:B:159:TRP:CZ3	2.48	0.47
1:B:406:LEU:O	1:B:406:LEU:HD12	2.14	0.47
1:B:172:LEU:HD22	1:B:177:GLY:C	2.40	0.47
1:B:253:HIS:CE1	1:B:308:ILE:O	2.67	0.47
1:B:323:GLN:O	1:B:326:LEU:O	2.32	0.47
1:B:479:VAL:HG21	1:B:498:PHE:CE2	2.50	0.47
1:A:176:ARG:NE	1:B:163:ARG:HH22	2.13	0.47
1:A:346:ASP:O	1:A:347:PRO:C	2.58	0.47
1:A:454:PHE:CE1	1:A:498:PHE:HE1	2.32	0.47
1:B:52:ARG:HG2	1:B:263:TRP:HD1	1.75	0.47
1:B:174:GLY:O	1:B:175:PRO:C	2.57	0.47
1:A:89:ASP:O	1:A:159:TRP:CE3	2.68	0.47
1:A:264:TRP:HH2	1:A:367:GLY:HA3	1.80	0.47
1:B:241:GLU:CD	1:B:359:GLU:HG3	2.39	0.46
1:B:294:ILE:CD1	1:B:308:ILE:HD11	2.45	0.46
1:B:473:LEU:HD21	1:B:489:ARG:HD3	1.95	0.46
1:A:5:LEU:HD12	1:A:5:LEU:HA	1.74	0.46
1:B:57:ARG:NH2	1:B:59:ASP:OD1	2.48	0.46
1:A:238:MET:SD	1:A:364:VAL:HG22	2.55	0.46
1:B:476:THR:HB	1:B:489:ARG:NH1	2.30	0.46
1:B:30:GLY:O	1:B:232:VAL:HB	2.14	0.46
1:B:461:ASP:HB2	1:B:473:LEU:CB	2.43	0.46
1:A:387:ARG:CZ	1:A:389:VAL:HG21	2.46	0.46
1:B:229:ILE:HG13	1:B:365:ASP:HB3	1.97	0.46
1:B:473:LEU:HD22	1:B:489:ARG:HD3	1.96	0.46
1:A:86:PRO:HA	1:A:164:TYR:HA	1.96	0.46
1:A:186:ARG:HD2	1:A:189:THR:HA	1.97	0.46
1:A:286:HIS:CG	1:A:287:TYR:H	2.34	0.46
1:A:346:ASP:HA	1:A:350:GLY:HA2	1.96	0.46
1:A:173:ARG:NH1	1:A:173:ARG:CB	2.70	0.46
1:A:230:PHE:CD2	1:A:300:HIS:CE1	3.04	0.46
1:A:346:ASP:O	1:A:346:ASP:CG	2.57	0.46
1:B:49:TRP:CZ2	1:B:238:MET:HB2	2.50	0.46
1:B:165:PHE:O	1:B:166:ASN:C	2.59	0.46
1:B:244:VAL:CG2	1:B:252:TRP:CD1	2.99	0.46
1:A:326:LEU:HD23	1:A:341:ARG:NH2	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HD2	2:A:1552:ATP:O2'	2.15	0.46
1:A:395:GLN:HB3	1:A:505:TRP:CZ2	2.51	0.46
1:B:49:TRP:CE2	1:B:238:MET:HB2	2.51	0.46
1:B:442:LYS:CA	1:B:445:ARG:HD3	2.32	0.46
1:A:231:ARG:HG2	1:A:231:ARG:O	2.16	0.46
1:A:310:GLN:CA	1:A:310:GLN:HE21	2.29	0.46
1:A:191:GLN:O	1:A:195:VAL:HG22	2.15	0.45
1:A:480:ARG:HG2	1:A:480:ARG:O	2.16	0.45
1:B:71:ARG:HH21	1:B:179:ARG:HH21	1.64	0.45
1:B:241:GLU:OE1	1:B:359:GLU:HG3	2.16	0.45
1:B:408:LYS:HE2	1:B:436:ASP:O	2.16	0.45
1:B:447:HIS:HA	1:B:450:VAL:HG22	1.98	0.45
1:A:260:ARG:HD3	1:A:306:GLU:OE2	2.16	0.45
1:A:295:LEU:N	1:A:295:LEU:CD2	2.80	0.45
1:B:86:PRO:HG3	1:B:164:TYR:CE1	2.50	0.45
1:B:408:LYS:HE2	1:B:437:THR:O	2.16	0.45
1:A:55:TYR:HE1	1:B:40:GLU:OE2	1.99	0.45
1:A:245:ARG:NH2	1:A:347:PRO:O	2.49	0.45
1:A:306:GLU:CD	1:A:362:ALA:HB2	2.41	0.45
1:A:323:GLN:HE22	1:A:334:ARG:CA	2.27	0.45
1:A:356:TYR:C	1:A:357:VAL:HG23	2.41	0.45
1:B:313:ASP:HB3	1:B:356:TYR:CD1	2.52	0.45
1:B:379:GLU:O	1:B:386:GLU:HA	2.17	0.45
1:B:447:HIS:HB3	1:B:452:THR:OG1	2.16	0.45
1:A:172:LEU:HD23	1:A:181:LEU:HD12	1.98	0.45
1:A:278:GLN:NE2	1:A:292:VAL:HG22	2.31	0.45
1:B:173:ARG:O	1:B:175:PRO:HD2	2.17	0.45
1:B:193:ILE:HD11	1:B:214:GLN:HB3	1.99	0.45
1:A:49:TRP:CH2	1:A:238:MET:HB2	2.52	0.45
1:A:263:TRP:NE1	1:A:267:MET:HE3	2.31	0.45
1:B:161:PRO:HA	1:B:162:PRO:HD2	1.68	0.45
1:A:52:ARG:O	1:A:52:ARG:HD3	2.16	0.45
1:A:259:GLU:O	1:A:262:LYS:HB3	2.17	0.45
1:A:447:HIS:HB3	1:A:452:THR:OG1	2.16	0.45
1:A:92:LYS:HD2	1:A:95:TYR:HE2	1.82	0.45
1:A:230:PHE:CE2	1:A:303:LEU:HD13	2.38	0.45
1:B:479:VAL:HG23	1:B:479:VAL:O	2.17	0.45
1:A:92:LYS:H	1:A:92:LYS:HG3	1.70	0.45
1:A:479:VAL:HG12	1:A:490:LEU:HD11	1.98	0.45
1:B:344:TYR:HD1	1:B:345:ARG:N	2.10	0.45
1:A:222:GLU:HG2	1:A:231:ARG:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PHE:CB	1:B:166:ASN:HA	2.47	0.45
1:B:219:PHE:CE2	1:B:234:GLU:OE1	2.71	0.44
1:B:224:THR:OG1	1:B:231:ARG:NH2	2.50	0.44
1:B:316:LEU:HD22	1:B:342:LEU:CG	2.41	0.44
1:B:456:VAL:HG11	1:B:495:LEU:HD21	1.99	0.44
1:B:9:VAL:HG22	1:B:228:PHE:CD2	2.53	0.44
1:B:187:PRO:HA	1:B:219:PHE:O	2.17	0.44
1:A:28:LEU:HB3	1:A:31:VAL:HG13	2.00	0.44
1:A:72:LEU:HD12	1:B:25:TYR:HB3	1.99	0.44
1:B:427:LEU:CD1	1:B:429:LEU:HD12	2.47	0.44
1:A:70:HIS:O	1:A:71:ARG:C	2.60	0.44
1:A:173:ARG:CZ	1:A:173:ARG:CA	2.95	0.44
1:A:289:LYS:HE2	1:A:310:GLN:OE1	2.17	0.44
1:A:15:ARG:HH21	1:A:449:GLU:HG3	1.80	0.44
1:A:167:MET:O	1:A:221:ASN:HB3	2.18	0.44
1:A:228:PHE:CG	1:A:229:ILE:N	2.85	0.44
1:A:399:ILE:O	1:A:452:THR:HB	2.18	0.44
1:A:406:LEU:CD2	1:A:459:ASP:HB2	2.48	0.44
1:A:434:TYR:CE1	1:A:436:ASP:HB3	2.52	0.44
1:B:401:VAL:CG1	1:B:456:VAL:HG23	2.47	0.44
1:A:18:ILE:CG2	1:A:32:TYR:HD2	2.31	0.44
1:A:42:LYS:HD3	1:A:46:LYS:CE	2.48	0.44
1:B:240:ILE:HB	1:B:360:PRO:HD2	2.00	0.44
1:A:328:ILE:CG2	1:A:329:THR:N	2.81	0.44
1:A:400:LYS:O	1:A:453:PRO:HG2	2.18	0.44
1:A:452:THR:HA	1:A:453:PRO:HD2	1.77	0.44
1:A:346:ASP:N	1:A:347:PRO:HD3	2.32	0.43
1:A:473:LEU:HD23	1:A:473:LEU:HA	1.79	0.43
1:B:387:ARG:CZ	1:B:485:MET:SD	3.06	0.43
1:B:498:PHE:CE1	1:B:502:ARG:CZ	3.00	0.43
1:A:72:LEU:HB3	1:B:25:TYR:CD2	2.53	0.43
1:A:172:LEU:HB3	1:A:181:LEU:HD12	2.00	0.43
1:A:252:TRP:O	1:A:255:TYR:HB3	2.18	0.43
1:B:253:HIS:HB2	1:B:310:GLN:HG3	2.00	0.43
1:B:279:GLN:HG3	1:B:291:THR:O	2.18	0.43
1:B:170:GLN:NE2	1:B:184:TYR:CE2	2.86	0.43
1:B:179:ARG:NE	1:B:182:LEU:HD22	2.33	0.43
1:B:275:VAL:HG23	1:B:295:LEU:HB2	2.01	0.43
1:B:452:THR:HA	1:B:453:PRO:HD3	1.82	0.43
1:A:73:VAL:HG13	1:A:319:HIS:CE1	2.54	0.43
1:A:237:GLN:NE2	1:A:239:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:THR:HG22	1:A:471:THR:H	1.82	0.43
1:A:230:PHE:HZ	1:A:303:LEU:HB3	1.82	0.43
1:A:498:PHE:CE1	1:A:502:ARG:HD3	2.53	0.43
1:B:34:TYR:CZ	1:B:42:LYS:HD3	2.53	0.43
1:B:265:GLN:NE2	1:B:271:ARG:HD3	2.33	0.43
1:A:223:ILE:HD13	1:A:223:ILE:HA	1.88	0.43
1:A:413:ILE:HG13	1:A:463:ILE:CD1	2.41	0.43
1:B:45:LEU:HD12	1:B:45:LEU:HA	1.83	0.43
1:B:221:ASN:O	1:B:221:ASN:OD1	2.37	0.43
1:B:416:TYR:HD1	1:B:416:TYR:O	2.02	0.43
1:A:5:LEU:HD22	1:A:300:HIS:HD2	1.84	0.43
1:A:317:GLY:C	1:A:319:HIS:H	2.26	0.43
1:B:88:VAL:O	1:B:159:TRP:CZ3	2.71	0.43
1:B:224:THR:O	1:B:231:ARG:NH2	2.49	0.43
1:B:306:GLU:HG3	1:B:361:SER:O	2.18	0.43
1:B:479:VAL:HG22	1:B:488:ILE:HG12	2.00	0.43
1:A:445:ARG:O	1:A:446:ARG:C	2.62	0.43
1:A:480:ARG:HD2	1:A:487:GLN:NE2	2.33	0.43
1:B:15:ARG:HD3	1:B:450:VAL:HG13	1.99	0.43
1:B:83:PHE:CE1	1:B:167:MET:HE2	2.54	0.43
1:B:241:GLU:OE2	1:B:359:GLU:HG3	2.19	0.43
1:A:29:GLN:O	1:A:233:ARG:NH1	2.52	0.43
1:B:381:LEU:HD11	1:B:387:ARG:HB3	2.00	0.43
1:A:169:PHE:CD2	1:A:219:PHE:HB3	2.54	0.42
1:A:87:MET:O	1:A:88:VAL:HG13	2.19	0.42
1:A:185:LEU:HD21	1:B:185:LEU:HD11	2.01	0.42
1:A:312:THR:O	1:A:356:TYR:CA	2.62	0.42
1:A:491:HIS:HD2	1:A:492:VAL:N	2.17	0.42
1:B:279:GLN:HA	1:B:280:PRO:HD3	1.73	0.42
1:B:416:TYR:CE1	1:B:420:LEU:HD22	2.54	0.42
1:A:241:GLU:CD	1:A:359:GLU:HG3	2.44	0.42
1:B:185:LEU:HD13	1:B:219:PHE:CD2	2.54	0.42
1:B:405:PRO:HA	1:B:458:VAL:HG23	2.02	0.42
1:B:423:ARG:O	1:B:426:ALA:HB3	2.19	0.42
1:B:52:ARG:CG	1:B:52:ARG:NH1	2.80	0.42
1:B:53:ASN:N	1:B:53:ASN:HD22	2.18	0.42
1:B:179:ARG:HD2	1:B:179:ARG:HA	1.74	0.42
1:A:326:LEU:H	1:A:326:LEU:HG	1.50	0.42
1:B:372:LEU:HA	1:B:372:LEU:HD23	1.64	0.42
1:B:390:LEU:HD13	1:B:392:LEU:CD1	2.50	0.42
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:CB	1:B:281:PRO:HD2	2.46	0.42
1:B:328:ILE:H	1:B:328:ILE:HG12	1.51	0.42
1:B:410:ARG:HB3	1:B:413:ILE:CD1	2.50	0.42
1:A:308:ILE:N	1:A:308:ILE:HD12	2.34	0.42
1:A:410:ARG:HE	1:A:460:TYR:HE1	1.55	0.42
1:A:415:GLU:C	1:A:419:ARG:HD3	2.44	0.42
1:B:479:VAL:CG2	1:B:488:ILE:HG12	2.50	0.42
1:A:49:TRP:CZ2	1:A:238:MET:HB2	2.55	0.42
1:A:310:GLN:HE21	1:A:310:GLN:C	2.28	0.42
1:A:344:TYR:HD2	1:A:353:PHE:CZ	2.38	0.42
1:A:367:GLY:O	1:A:371:LEU:HG	2.20	0.42
1:B:196:ASN:O	1:B:197:PHE:C	2.62	0.42
1:B:242:TYR:HD2	1:B:244:VAL:CG2	2.32	0.42
1:B:249:ASP:OD1	1:B:250:GLU:N	2.53	0.42
1:A:40:GLU:O	1:A:41:LEU:C	2.63	0.41
1:B:83:PHE:CD1	1:B:167:MET:HE2	2.55	0.41
1:B:223:ILE:HD12	1:B:223:ILE:HA	1.75	0.41
1:B:459:ASP:O	1:B:462:THR:N	2.53	0.41
1:A:415:GLU:OE2	1:A:419:ARG:HD2	2.20	0.41
1:B:393:LYS:HD3	1:B:394:PRO:HD2	2.02	0.41
1:A:30:GLY:O	1:A:232:VAL:HB	2.20	0.41
1:A:208:LEU:O	1:A:209:GLY:C	2.60	0.41
1:A:265:GLN:NE2	1:A:271:ARG:HD3	2.35	0.41
1:A:321:LYS:H	1:A:341:ARG:HA	1.84	0.41
1:B:290:ALA:C	1:B:291:THR:HG22	2.45	0.41
1:B:473:LEU:HA	1:B:473:LEU:HD23	1.74	0.41
1:B:476:THR:HG23	1:B:490:LEU:C	2.44	0.41
1:A:175:PRO:HD3	1:B:223:ILE:CD1	2.49	0.41
1:A:198:LYS:HD2	1:A:202:ASP:OD1	2.20	0.41
1:A:321:LYS:NZ	1:A:321:LYS:HB3	2.35	0.41
1:A:387:ARG:CZ	1:A:389:VAL:CG2	2.98	0.41
1:B:72:LEU:O	1:B:73:VAL:C	2.63	0.41
1:B:313:ASP:HB3	1:B:356:TYR:CE1	2.54	0.41
1:A:94:ARG:HH12	1:B:176:ARG:HG3	1.84	0.41
1:A:287:TYR:H	1:A:287:TYR:HD1	1.68	0.41
1:B:40:GLU:HB2	1:B:398:PRO:HB3	2.02	0.41
1:B:63:LEU:HD23	1:B:214:GLN:NE2	2.35	0.41
1:A:218:ALA:HB3	1:A:235:PHE:CE1	2.56	0.41
1:A:264:TRP:CH2	1:A:367:GLY:HA3	2.55	0.41
1:A:310:GLN:O	1:A:310:GLN:CG	2.69	0.41
1:A:317:GLY:C	1:A:319:HIS:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLN:HG2	1:A:505:TRP:CG	2.56	0.41
1:A:443:ALA:O	1:A:444:TYR:C	2.63	0.41
1:B:306:GLU:CD	1:B:362:ALA:HB2	2.46	0.41
1:A:14:ARG:O	1:A:15:ARG:HD3	2.20	0.41
1:A:347:PRO:HD3	1:A:351:LYS:O	2.21	0.41
1:A:387:ARG:HD2	1:A:445:ARG:NH2	2.22	0.41
1:A:445:ARG:O	1:A:445:ARG:HD3	2.21	0.41
1:B:12:CYS:HA	1:B:17:PHE:HB2	2.03	0.41
1:B:461:ASP:OD1	1:B:462:THR:N	2.54	0.41
1:B:297:ARG:NE	1:B:302:SER:HB2	2.36	0.41
1:B:323:GLN:HE22	1:B:335:ASN:H	1.65	0.41
1:B:378:ARG:HB3	1:B:386:GLU:OE1	2.21	0.41
1:A:161:PRO:HA	1:A:162:PRO:HD3	1.92	0.41
1:A:438:GLY:O	1:A:439:ASN:C	2.63	0.41
1:B:163:ARG:HE	1:B:163:ARG:HB3	1.62	0.41
1:B:324:GLU:HB3	1:B:334:ARG:NH1	2.36	0.41
1:B:363:GLY:CA	2:B:2552:ATP:H1'	2.50	0.41
1:B:461:ASP:O	1:B:474:LYS:HA	2.20	0.41
1:A:21:SER:HB3	1:A:31:VAL:HG22	2.03	0.41
1:A:176:ARG:HE	1:B:163:ARG:NH1	2.14	0.41
1:A:275:VAL:HB	1:A:295:LEU:HB2	2.03	0.41
1:B:297:ARG:CZ	1:B:302:SER:CB	2.99	0.41
1:B:311:ARG:HB2	1:B:357:VAL:HG13	2.03	0.41
1:A:187:PRO:HG2	1:A:188:GLU:HG2	2.03	0.40
1:B:8:LEU:HD13	1:B:8:LEU:HA	1.88	0.40
1:B:252:TRP:O	1:B:255:TYR:HB3	2.21	0.40
1:A:328:ILE:HG22	1:A:329:THR:N	2.36	0.40
1:A:410:ARG:HA	1:A:411:PRO:HD2	1.73	0.40
1:B:53:ASN:O	1:B:57:ARG:HG3	2.21	0.40
1:B:193:ILE:HD12	1:B:241:GLU:HG2	2.03	0.40
1:A:200:VAL:O	1:A:204:THR:HG23	2.21	0.40
1:A:221:ASN:O	1:A:221:ASN:CG	2.63	0.40
1:A:306:GLU:HG3	1:A:361:SER:O	2.22	0.40
1:B:90:ASN:CG	1:B:91:ALA:N	2.79	0.40
1:A:237:GLN:HE22	1:A:239:GLU:CD	2.28	0.40
1:A:298:PHE:O	1:A:299:PRO:C	2.65	0.40
1:A:495:LEU:O	1:A:499:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/442 (99%)	355 (81%)	65 (15%)	18 (4%)	2	15
1	B	438/442 (99%)	354 (81%)	63 (14%)	21 (5%)	2	11
All	All	876/884 (99%)	709 (81%)	128 (15%)	39 (4%)	2	12

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	PRO
1	A	281	PRO
1	A	286	HIS
1	A	438	GLY
1	B	92	LYS
1	B	175	PRO
1	B	227	ASN
1	B	281	PRO
1	B	284	SER
1	B	286	HIS
1	B	438	GLY
1	A	209	GLY
1	A	284	SER
1	A	327	GLY
1	A	349	THR
1	B	209	GLY
1	B	229	ILE
1	B	339	THR
1	B	439	ASN
1	B	468	ASP
1	A	79	HIS
1	A	350	GLY
1	A	439	ASN
1	A	470	THR
1	B	166	ASN

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Mol	Chain	Res	Type
1	B	276	PRO
1	B	302	SER
1	A	71	ARG
1	A	382	PRO
1	B	221	ASN
1	A	174	GLY
1	A	227	ASN
1	B	246	PRO
1	B	337	HIS
1	A	276	PRO
1	B	174	GLY
1	B	36	PRO
1	B	440	ILE
1	A	246	PRO

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	375/376 (100%)	312 (83%)	63 (17%)	2	9
1	B	374/376 (100%)	307 (82%)	67 (18%)	2	7
All	All	749/752 (100%)	619 (83%)	130 (17%)	2	8

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	20	GLN
1	A	31	VAL
1	A	36	PRO
1	A	60	MET
1	A	66	SER
1	A	72	LEU
1	A	85	ASP
1	A	88	VAL

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Mol	Chain	Res	Type
1	A	92	LYS
1	A	162	PRO
1	A	173	ARG
1	A	175	PRO
1	A	189	THR
1	A	193	ILE
1	A	208	LEU
1	A	210	PHE
1	A	222	GLU
1	A	223	ILE
1	A	226	ARG
1	A	237	GLN
1	A	238	MET
1	A	246	PRO
1	A	258	GLU
1	A	261	LEU
1	A	262	LYS
1	A	272	GLU
1	A	291	THR
1	A	295	LEU
1	A	303	LEU
1	A	310	GLN
1	A	311	ARG
1	A	321	LYS
1	A	324	GLU
1	A	326	LEU
1	A	331	ARG
1	A	345	ARG
1	A	351	LYS
1	A	369	LEU
1	A	390	LEU
1	A	392	LEU
1	A	398	PRO
1	A	407	VAL
1	A	410	ARG
1	A	412	GLU
1	A	415	GLU
1	A	421	LYS
1	A	423	ARG
1	A	442	LYS
1	A	449	GLU
1	A	457	THR

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Mol	Chain	Res	Type
1	A	462	THR
1	A	467	LYS
1	A	471	THR
1	A	472	ARG
1	A	477	VAL
1	A	478	THR
1	A	479	VAL
1	A	488	ILE
1	A	490	LEU
1	A	501	GLU
1	A	502	ARG
1	A	504	ARG
1	B	3	SER
1	B	5	LEU
1	B	6	ASP
1	B	15	ARG
1	B	28	LEU
1	B	36	PRO
1	B	37	LEU
1	B	39	VAL
1	B	46	LYS
1	B	52	ARG
1	B	63	LEU
1	B	72	LEU
1	B	94	ARG
1	B	163	ARG
1	B	167	MET
1	B	168	MET
1	B	170	GLN
1	B	173	ARG
1	B	175	PRO
1	B	193	ILE
1	B	205	SER
1	B	208	LEU
1	B	219	PHE
1	B	223	ILE
1	B	228	PHE
1	B	238	MET
1	B	239	GLU
1	B	246	PRO
1	B	254	ARG
1	B	275	VAL

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Mol	Chain	Res	Type
1	B	282	GLU
1	B	284	SER
1	B	291	THR
1	B	297	ARG
1	B	303	LEU
1	B	305	LEU
1	B	310	GLN
1	B	328	ILE
1	B	331	ARG
1	B	333	LEU
1	B	340	GLN
1	B	345	ARG
1	B	357	VAL
1	B	369	LEU
1	B	376	PHE
1	B	385	GLU
1	B	386	GLU
1	B	398	PRO
1	B	400	LYS
1	B	406	LEU
1	B	409	ASN
1	B	412	GLU
1	B	420	LEU
1	B	431	ARG
1	B	433	LEU
1	B	440	ILE
1	B	467	LYS
1	B	470	THR
1	B	477	VAL
1	B	478	THR
1	B	485	MET
1	B	487	GLN
1	B	488	ILE
1	B	490	LEU
1	B	496	GLU
1	B	498	PHE
1	B	502	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN

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Mol	Chain	Res	Type
1	A	166	ASN
1	A	196	ASN
1	A	199	ASN
1	A	221	ASN
1	A	227	ASN
1	A	237	GLN
1	A	278	GLN
1	A	300	HIS
1	A	323	GLN
1	A	335	ASN
1	A	487	GLN
1	A	491	HIS
1	B	44	ASN
1	B	75	HIS
1	B	90	ASN
1	B	170	GLN
1	B	196	ASN
1	B	214	GLN
1	B	221	ASN
1	B	227	ASN
1	B	237	GLN
1	B	253	HIS
1	B	323	GLN
1	B	340	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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	A	1552	-	32,33,33	1.06	3 (9%)	48,52,52	0.61	0
2	ATP	B	2552	-	32,33,33	0.85	2 (6%)	48,52,52	0.58	0

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	ATP	A	1552	-	-	5/22/38/38	0/3/3/3
2	ATP	B	2552	-	-	4/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1552	ATP	PB-O3B	3.53	1.63	1.59
2	A	1552	ATP	PB-O3A	3.28	1.63	1.59
2	B	2552	ATP	PB-O3B	3.26	1.63	1.59
2	A	1552	ATP	PA-O3A	2.48	1.62	1.59
2	B	2552	ATP	PB-O3A	2.03	1.61	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1552	ATP	PB-O3A-PA-O5'
2	A	1552	ATP	C5'-O5'-PA-O2A
2	A	1552	ATP	C5'-O5'-PA-O3A
2	B	2552	ATP	PB-O3A-PA-O5'
2	B	2552	ATP	PB-O3B-PG-O1G
2	A	1552	ATP	PA-O3A-PB-O1B

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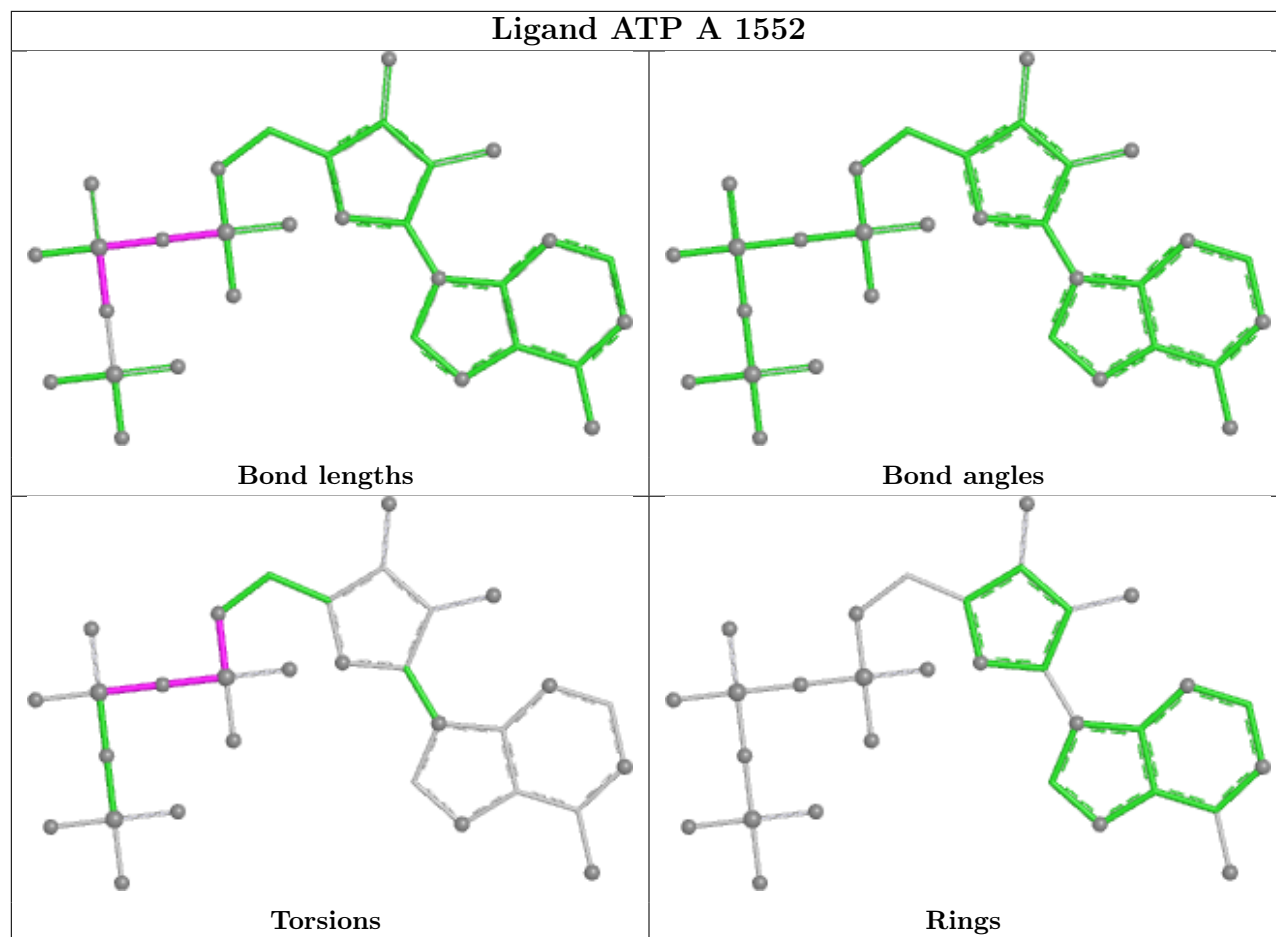
Mol	Chain	Res	Type	Atoms
2	B	2552	ATP	PB-O3B-PG-O2G
2	B	2552	ATP	PB-O3B-PG-O3G
2	A	1552	ATP	PA-O3A-PB-O2B

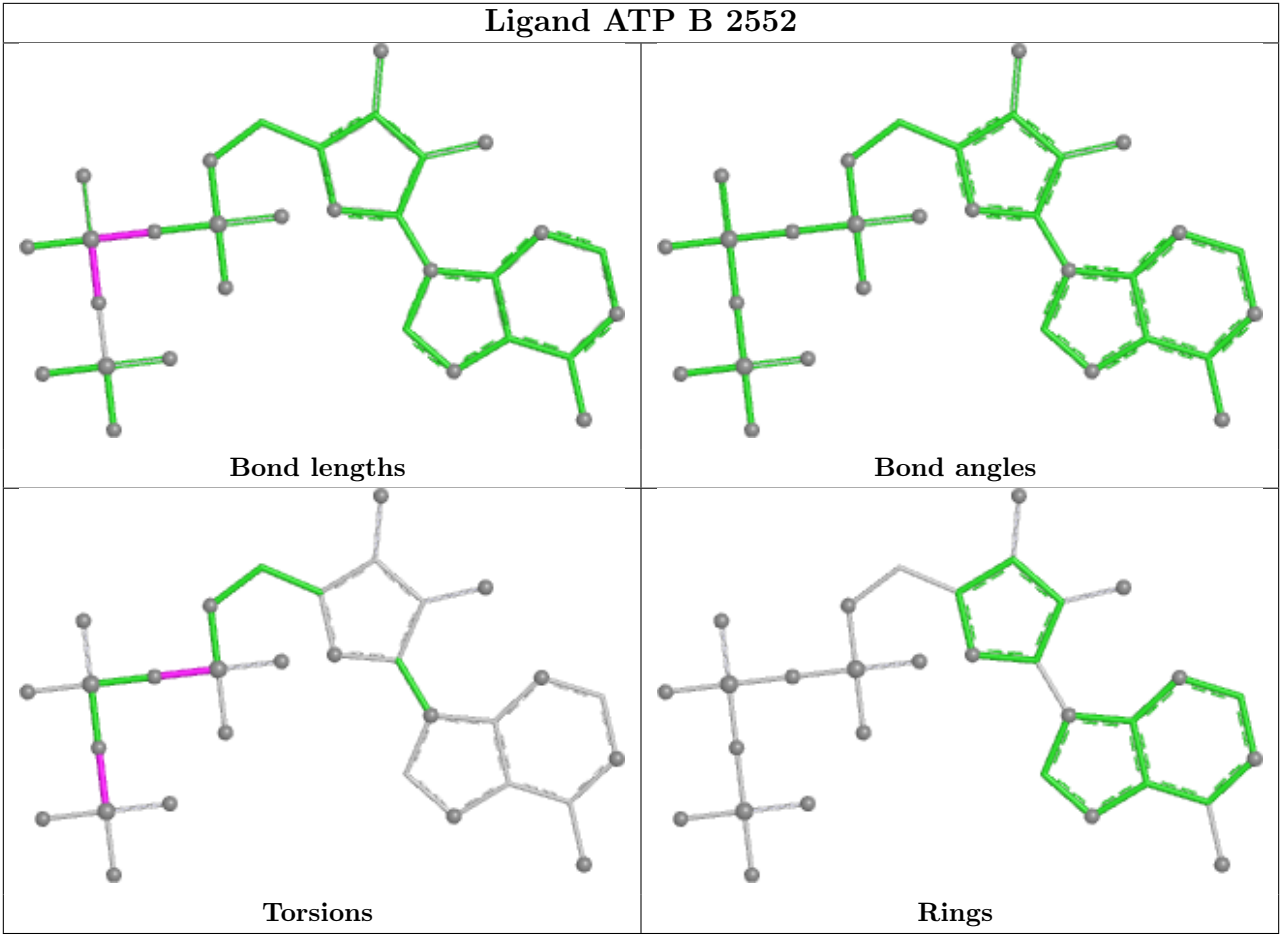
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1552	ATP	5	0
2	B	2552	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	95:TYR	C	159:TRP	N	11.48
1	B	95:TYR	C	159:TRP	N	11.20

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	442/442 (100%)	0.99	65 (14%) 6 7	12, 31, 61, 93	0
1	B	442/442 (100%)	1.20	88 (19%) 3 4	12, 33, 65, 90	0
All	All	884/884 (100%)	1.10	153 (17%) 4 5	12, 32, 64, 93	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ALA	10.7
1	B	85	ASP	6.8
1	B	335	ASN	6.5
1	B	209	GLY	5.2
1	B	183	ALA	4.8
1	A	448	ASP	4.8
1	B	62	GLY	4.7
1	B	174	GLY	4.5
1	A	25	TYR	4.5
1	B	285	ALA	4.4
1	B	330	ALA	4.4
1	B	318	SER	4.4
1	B	284	SER	4.4
1	B	338	SER	4.3
1	B	286	HIS	4.2
1	A	349	THR	4.2
1	B	253	HIS	4.1
1	A	445	ARG	4.0
1	B	466	SER	4.0
1	A	441	GLY	3.9
1	B	54	VAL	3.9
1	A	286	HIS	3.8
1	B	224	THR	3.8
1	A	383	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	361	SER	3.8
1	B	381	LEU	3.8
1	B	246	PRO	3.7
1	A	373	ALA	3.7
1	A	461	ASP	3.7
1	A	10	ALA	3.7
1	A	375	ALA	3.6
1	B	90	ASN	3.6
1	B	322	ASP	3.6
1	B	346	ASP	3.6
1	A	384	GLY	3.5
1	B	327	GLY	3.5
1	A	20	GLN	3.5
1	B	332	VAL	3.5
1	A	470	THR	3.4
1	A	347	PRO	3.4
1	B	89	ASP	3.4
1	A	474	LYS	3.4
1	A	493	ASP	3.2
1	A	283	SER	3.2
1	B	461	ASP	3.2
1	A	224	THR	3.2
1	B	329	THR	3.2
1	A	285	ALA	3.1
1	B	202	ASP	3.1
1	B	249	ASP	3.0
1	A	16	GLY	2.9
1	B	385	GLU	2.9
1	A	370	ALA	2.8
1	B	167	MET	2.8
1	B	91	ALA	2.8
1	B	221	ASN	2.8
1	A	172	LEU	2.8
1	B	464	GLY	2.8
1	A	422	ALA	2.8
1	B	350	GLY	2.8
1	B	75	HIS	2.8
1	B	280	PRO	2.8
1	B	80	GLU	2.8
1	B	208	LEU	2.8
1	A	389	VAL	2.7
1	A	413	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	44	ASN	2.7
1	A	159	TRP	2.7
1	B	302	SER	2.7
1	B	242	TYR	2.7
1	B	383	ASN	2.7
1	A	225	PRO	2.6
1	A	411	PRO	2.6
1	B	4	SER	2.6
1	A	88	VAL	2.6
1	A	443	ALA	2.6
1	B	49	TRP	2.6
1	B	323	GLN	2.6
1	B	159	TRP	2.6
1	B	345	ARG	2.6
1	A	26	GLY	2.6
1	A	171	ASP	2.6
1	A	254	ARG	2.6
1	A	160	THR	2.6
1	A	462	THR	2.6
1	A	92	LYS	2.5
1	A	335	ASN	2.5
1	A	394	PRO	2.5
1	B	188	GLU	2.5
1	B	463	ILE	2.5
1	A	350	GLY	2.5
1	B	84	ALA	2.5
1	B	227	ASN	2.5
1	B	347	PRO	2.5
1	B	356	TYR	2.5
1	A	463	ILE	2.5
1	A	89	ASP	2.5
1	A	476	THR	2.5
1	A	481	ASP	2.4
1	B	427	LEU	2.4
1	B	344	TYR	2.4
1	B	473	LEU	2.4
1	B	69	THR	2.4
1	B	199	ASN	2.4
1	A	408	LYS	2.4
1	A	11	LEU	2.4
1	B	73	VAL	2.4
1	B	65	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	324	GLU	2.4
1	A	385	GLU	2.4
1	A	192	GLY	2.3
1	B	291	THR	2.3
1	A	71	ARG	2.3
1	B	357	VAL	2.3
1	B	290	ALA	2.3
1	B	328	ILE	2.3
1	B	171	ASP	2.3
1	B	279	GLN	2.3
1	A	415	GLU	2.3
1	B	325	ALA	2.3
1	B	189	THR	2.3
1	A	90	ASN	2.3
1	A	494	GLU	2.2
1	B	411	PRO	2.2
1	B	21	SER	2.2
1	A	9	VAL	2.2
1	B	251	TYR	2.2
1	A	181	LEU	2.2
1	B	317	GLY	2.2
1	B	349	THR	2.2
1	A	410	ARG	2.2
1	B	45	LEU	2.1
1	A	500	ARG	2.1
1	B	353	PHE	2.1
1	A	7	GLU	2.1
1	B	207	LYS	2.1
1	B	419	ARG	2.1
1	A	465	GLN	2.1
1	A	4	SER	2.1
1	B	165	PHE	2.1
1	A	221	ASN	2.1
1	B	203	ALA	2.1
1	B	278	GLN	2.1
1	B	415	GLU	2.1
1	B	83	PHE	2.1
1	B	194	PHE	2.1
1	B	259	GLU	2.1
1	A	5	LEU	2.0
1	B	337	HIS	2.0
1	B	476	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	19	PHE	2.0
1	B	243	PHE	2.0
1	A	14	ARG	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](#)

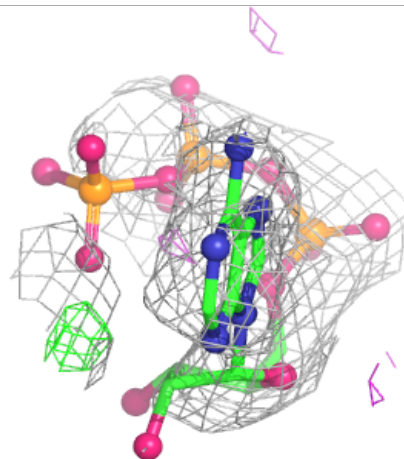
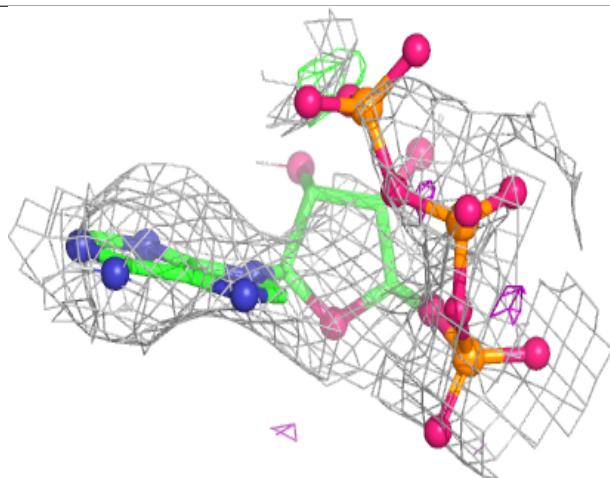
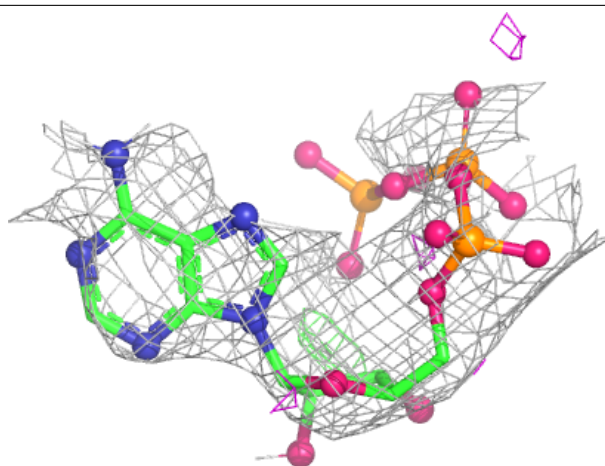
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

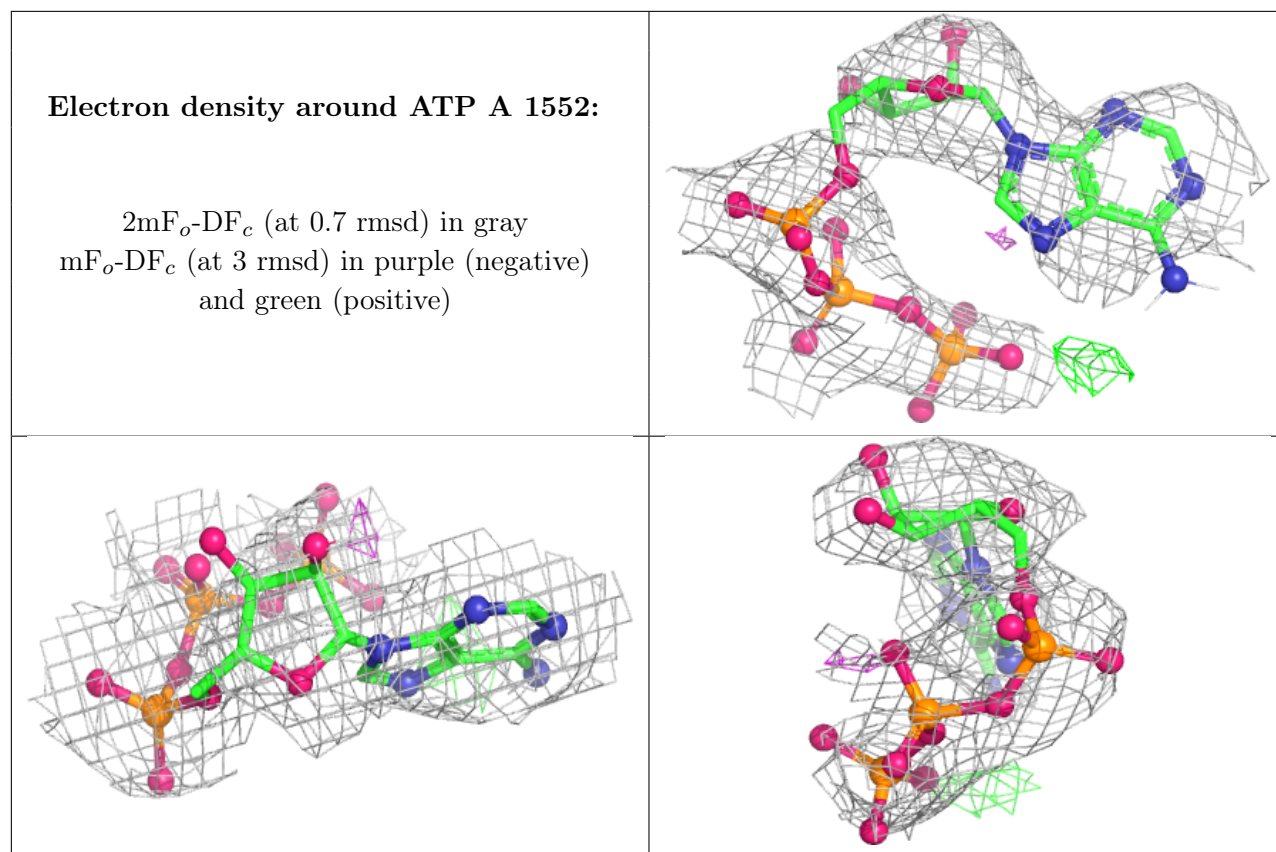
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	B	2552	31/31	0.80	0.19	0,67,102,102	0
2	ATP	A	1552	31/31	0.90	0.15	0,42,82,84	0

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 ATP B 2552:

$2mF_o-DF_c$ (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.