



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:21 AM UTC

PDB ID : 2P9S / pdb_00002p9s
Title : Structure of bovine Arp2/3 complex co-crystallized with ATP/Mg2+
Authors : Nolen, B.J.; Pollard, T.D.
Deposited on : 2007-03-26
Resolution : 2.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

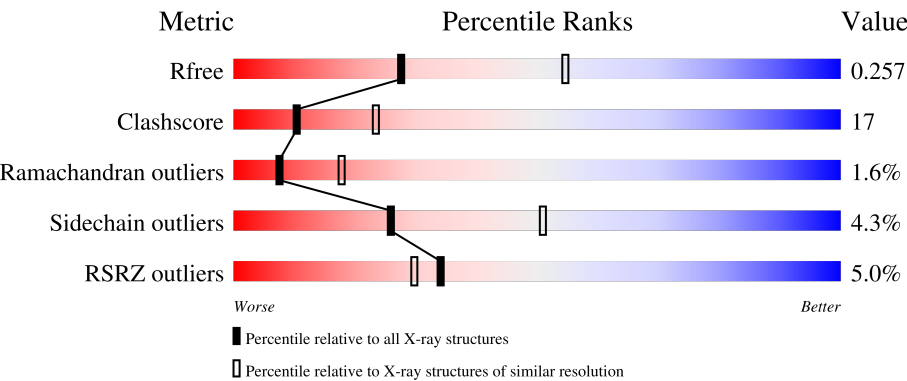
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	418	6% 68%22%5%
2	B	394	6% 29%19%50%
3	C	372	2% 59%30%8%
4	D	300	2% 67%24%7%
5	E	178	3% 53%38%5%

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Mol	Chain	Length	Quality of chain
6	F	168	% 75% 23% ...
7	G	151	11% 58% 25% 6% 11%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13608 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 Actin-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3125	2006	517	587	15			

- Molecule 2 is a protein called Actin-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1487	951	251	281	4			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	341	Total	C	N	O	S	0	0	0
			2641	1676	463	483	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	VAL	ILE	conflict	UNP Q58CQ2

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	280	Total	C	N	O	S	0	0	0
			2249	1430	392	419	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	173	Total	C	N	O	S	0	0	0
			1411	906	235	261	9			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1371	875	239	248	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	135	Total	C	N	O	S	0	0	0
			1028	643	177	205	3			

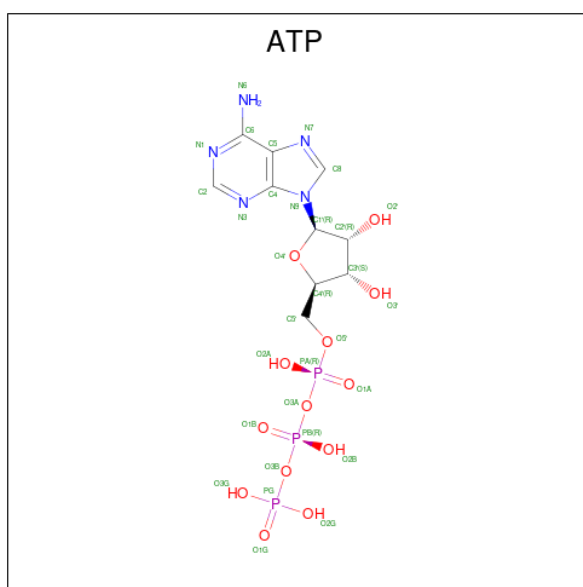
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	ASP	GLY	conflict	UNP Q3SYX9
G	28	ASP	GLU	conflict	UNP Q3SYX9

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
9	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 10 is water.

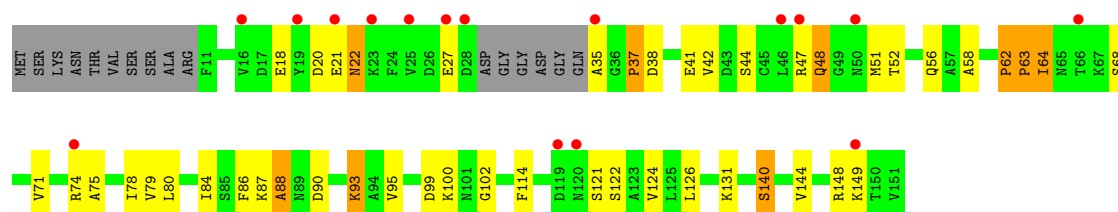
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	50	Total	O	0	0
			50	50		
10	B	15	Total	O	0	0
			15	15		
10	C	61	Total	O	0	0
			61	61		
10	D	47	Total	O	0	0
			47	47		
10	E	14	Total	O	0	0
			14	14		
10	F	39	Total	O	0	0
			39	39		
10	G	7	Total	O	0	0
			7	7		

Chain F:  %



• Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.02Å 128.69Å 201.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.68 30.00 – 2.68	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-2.68) 95.1 (30.00-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	10.40	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.261 0.220 , 0.257	Depositor DCC
R_{free} test set	4068 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13608	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: MG, 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	0.49	0/3205	0.97	12/4358 (0.3%)
2	B	0.43	0/1514	0.90	3/2059 (0.1%)
3	C	0.44	0/2710	1.01	12/3680 (0.3%)
4	D	0.47	0/2297	0.93	8/3101 (0.3%)
5	E	0.40	0/1445	1.00	9/1949 (0.5%)
6	F	0.46	0/1393	0.92	2/1868 (0.1%)
7	G	0.39	0/1040	0.92	5/1401 (0.4%)
All	All	0.45	0/13604	0.96	51/18416 (0.3%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	30	HIS	N-CA-C	-10.94	98.64	113.30
3	C	283	GLY	N-CA-C	9.86	128.86	112.30
1	A	155	SER	N-CA-C	9.64	131.34	110.80
4	D	83	TYR	N-CA-C	-7.44	104.01	113.23
7	G	22	ASN	N-CA-C	-7.09	103.66	114.16
1	A	97	ILE	N-CA-C	6.93	117.05	110.74
5	E	22	LEU	CA-C-N	6.91	126.83	119.85
5	E	22	LEU	C-N-CA	6.91	126.83	119.85
1	A	238	LEU	N-CA-C	6.90	118.50	110.97
5	E	63	GLU	N-CA-C	-6.90	104.73	113.01
1	A	109	TYR	N-CA-C	-6.82	100.39	110.48
1	A	76	TRP	CA-C-N	6.80	126.50	119.56
1	A	76	TRP	C-N-CA	6.80	126.50	119.56
3	C	137	ILE	N-CA-C	-6.52	97.72	107.37
6	F	109	VAL	N-CA-C	-6.49	101.22	109.58
4	D	244	ILE	N-CA-C	6.38	117.90	110.62
3	C	63	ASP	N-CA-C	6.38	118.03	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	79	VAL	N-CA-C	6.37	116.51	110.53
1	A	118	ASN	N-CA-C	-6.29	101.11	110.23
3	C	11	ILE	N-CA-C	-6.18	98.08	106.85
2	B	216	ILE	N-CA-C	-6.05	104.84	110.53
5	E	148	VAL	N-CA-C	6.04	116.82	110.72
4	D	123	SER	N-CA-C	6.02	118.33	111.11
1	A	153	TRP	N-CA-C	-6.01	105.66	112.87
7	G	148	ARG	N-CA-C	-5.99	106.11	113.41
1	A	154	THR	O-C-N	5.93	129.16	122.22
3	C	18	LYS	N-CA-C	5.78	117.26	111.07
3	C	46	HIS	N-CA-C	5.76	118.04	108.99
3	C	178	GLU	N-CA-C	5.71	117.78	108.76
3	C	161	SER	N-CA-C	5.67	117.58	109.14
5	E	26	SER	N-CA-C	5.64	117.84	108.99
7	G	140	SER	N-CA-C	-5.64	105.90	112.89
4	D	159	ASP	N-CA-C	5.55	116.96	110.41
5	E	84	LYS	N-CA-C	5.51	119.11	112.93
5	E	19	MET	N-CA-C	-5.50	101.89	110.42
4	D	129	PHE	N-CA-C	-5.47	105.48	111.82
2	B	220	LEU	N-CA-C	5.42	121.31	114.31
4	D	206	PRO	N-CA-C	-5.38	103.00	111.34
6	F	30	VAL	N-CA-C	5.28	115.50	108.11
1	A	373	GLN	N-CA-C	5.25	120.04	111.37
3	C	165	LYS	N-CA-C	5.25	118.05	109.59
2	B	227	ILE	N-CA-C	5.23	115.85	110.36
1	A	368	ILE	N-CA-C	5.22	116.22	108.23
5	E	109	PRO	N-CA-C	-5.18	103.14	111.38
3	C	253	ILE	N-CA-C	-5.17	108.24	113.47
4	D	33	VAL	N-CA-C	5.16	115.70	108.17
5	E	156	PRO	N-CA-C	-5.15	101.85	112.47
3	C	9	GLU	N-CA-C	-5.07	103.57	110.36
7	G	62	PRO	CA-C-N	5.07	126.17	119.84
7	G	62	PRO	C-N-CA	5.07	126.17	119.84
1	A	413	VAL	N-CA-C	-5.04	103.09	109.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3125	0	3001	92	0
2	B	1487	0	1440	57	0
3	C	2641	0	2589	105	0
4	D	2249	0	2206	65	0
5	E	1411	0	1413	77	0
6	F	1371	0	1410	36	0
7	G	1028	0	1029	32	0
8	A	1	0	0	0	0
9	A	31	0	12	2	0
9	B	31	0	12	3	0
10	A	50	0	0	2	0
10	B	15	0	0	0	0
10	C	61	0	0	1	0
10	D	47	0	0	1	0
10	E	14	0	0	0	0
10	F	39	0	0	0	0
10	G	7	0	0	0	0
All	All	13608	0	13112	449	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 17.

All (449) 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)
3:C:216:ARG:HG2	3:C:230:ASP:HB3	1.32	1.10
3:C:183:THR:HG22	3:C:185:TRP:H	1.24	1.01
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.45	0.99
3:C:14:HIS:H	3:C:331:GLN:HE22	1.07	0.91
3:C:201:SER:HB3	7:G:149:LYS:HZ2	1.35	0.91
3:C:201:SER:HB3	7:G:149:LYS:NZ	1.90	0.87
2:B:182:LEU:HD22	2:B:184:ILE:HG22	1.57	0.86
1:A:239:VAL:HG11	5:E:48:TYR:HD1	1.42	0.84
1:A:257:THR:HG22	1:A:268:SER:HB3	1.61	0.83
3:C:107:ASN:ND2	3:C:109:LYS:H	1.76	0.83
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.63	0.80
3:C:29:ASN:HB3	3:C:31:GLU:H	1.47	0.80
1:A:246:ASP:OD1	5:E:50:LYS:HE3	1.82	0.79
6:F:130:LYS:HA	6:F:130:LYS:HE2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:C	1:A:264:LYS:H	1.90	0.78
5:E:86:ASN:HB3	5:E:154:ASP:OD1	1.84	0.78
1:A:154:THR:O	1:A:155:SER:HB2	1.84	0.77
3:C:107:ASN:C	3:C:107:ASN:HD22	1.91	0.77
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.64	0.77
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.66	0.76
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.69	0.75
6:F:20:LEU:HD23	6:F:70:VAL:HG21	1.68	0.75
1:A:216:PRO:HB2	1:A:219:GLN:HB2	1.67	0.75
3:C:14:HIS:N	3:C:331:GLN:HE22	1.84	0.74
5:E:150:ASP:C	5:E:152:GLN:H	1.96	0.74
3:C:14:HIS:H	3:C:331:GLN:NE2	1.86	0.73
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.67	0.73
5:E:88:LYS:H	5:E:153:ASN:ND2	1.87	0.73
7:G:51:MET:HG3	7:G:87:LYS:NZ	2.04	0.72
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.70	0.72
4:D:137:GLU:OE2	4:D:158:LYS:HE2	1.89	0.72
3:C:17:ASN:ND2	3:C:22:GLN:HG3	2.05	0.72
3:C:179:ARG:HG3	3:C:179:ARG:HH11	1.54	0.72
6:F:2:THR:HG23	6:F:3:ALA:H	1.56	0.71
1:A:311:VAL:C	1:A:314:PRO:HD2	2.17	0.70
2:B:166:ILE:HD12	2:B:281:LEU:CD2	2.21	0.70
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.54	0.70
4:D:197:GLN:NE2	4:D:199:LEU:HD11	2.07	0.70
1:A:321:LEU:HD12	1:A:369:THR:HG22	1.75	0.69
3:C:216:ARG:HG2	3:C:230:ASP:CB	2.18	0.68
3:C:34:ILE:HB	3:C:46:HIS:HB2	1.74	0.68
3:C:284:ARG:NH1	3:C:286:ASP:O	2.25	0.68
4:D:266:MET:HE3	6:F:93:PHE:CD1	2.29	0.68
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.74	0.68
3:C:183:THR:HG22	3:C:185:TRP:N	2.05	0.67
2:B:318:GLU:HG3	2:B:344:ILE:HD12	1.75	0.67
7:G:38:ASP:O	7:G:42:VAL:HG23	1.95	0.66
1:A:262:ILE:O	1:A:264:LYS:N	2.28	0.66
3:C:107:ASN:HD22	3:C:108:GLU:N	1.93	0.66
3:C:269:LEU:H	3:C:283:GLY:HA2	1.61	0.66
2:B:218:GLU:HG2	9:B:502:ATP:C5	2.30	0.66
5:E:152:GLN:HB3	5:E:155:LYS:NZ	2.11	0.66
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.25	0.66
1:A:152:SER:C	1:A:154:THR:N	2.52	0.66
6:F:4:THR:HG23	6:F:55:ARG:HE	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:CG	4:D:264:THR:HG22	2.22	0.65
1:A:239:VAL:HG22	5:E:4:TYR:CZ	2.31	0.65
1:A:87:ASP:OD2	4:D:264:THR:HG22	1.97	0.65
2:B:230:GLU:OE2	6:F:35:LYS:HE3	1.97	0.65
1:A:327:MET:HE2	1:A:374:ARG:HB2	1.79	0.64
5:E:22:LEU:HD23	5:E:41:ILE:HB	1.78	0.64
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.31	0.64
5:E:150:ASP:C	5:E:152:GLN:N	2.55	0.64
5:E:76:SER:O	5:E:80:LYS:HG3	1.98	0.64
1:A:239:VAL:HG11	5:E:48:TYR:CD1	2.30	0.64
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.80	0.64
5:E:20:ALA:HB1	5:E:22:LEU:HD13	1.80	0.63
3:C:183:THR:HG23	3:C:184:PRO:CD	2.29	0.63
2:B:153:THR:CB	2:B:171:GLU:H	2.12	0.63
4:D:206:PRO:HD3	4:D:222:TYR:CG	2.33	0.63
1:A:152:SER:C	1:A:154:THR:H	2.06	0.63
7:G:121:SER:O	7:G:124:VAL:HG12	2.00	0.62
5:E:16:ILE:HG23	5:E:16:ILE:O	2.00	0.62
5:E:95:MET:HE3	5:E:95:MET:HA	1.81	0.62
5:E:24:ILE:HD11	5:E:135:GLN:HG2	1.81	0.62
4:D:228:PHE:H	4:D:231:HIS:HD2	1.48	0.62
1:A:343:VAL:HG13	1:A:363:ILE:HD12	1.82	0.61
5:E:150:ASP:O	5:E:152:GLN:N	2.34	0.61
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.36	0.61
1:A:262:ILE:C	1:A:264:LYS:N	2.58	0.61
5:E:95:MET:HG2	5:E:141:GLY:O	2.01	0.61
2:B:205:ASN:HD22	2:B:208:ALA:H	1.48	0.60
5:E:9:MET:HE2	5:E:13:THR:HB	1.83	0.60
6:F:2:THR:C	6:F:4:THR:H	2.09	0.60
3:C:229:ALA:HB2	3:C:237:VAL:HG22	1.83	0.60
6:F:101:PHE:O	6:F:103:ILE:N	2.35	0.60
3:C:142:ARG:HG3	3:C:142:ARG:HH11	1.66	0.60
3:C:281:PHE:CE1	3:C:283:GLY:HA3	2.36	0.60
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.84	0.60
1:A:164:THR:HA	1:A:180:VAL:O	2.03	0.59
4:D:233:ASN:O	4:D:237:ARG:HB2	2.01	0.59
3:C:370:LYS:O	3:C:371:ILE:HB	2.02	0.59
5:E:25:ARG:HH11	5:E:25:ARG:HG2	1.67	0.59
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.28	0.59
1:A:154:THR:CG2	1:A:370:HIS:HB2	2.33	0.59
3:C:21:THR:HG22	3:C:22:GLN:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:PHE:O	6:F:102:PHE:CD1	2.56	0.59
3:C:189:MET:HA	3:C:195:MET:HE1	1.85	0.58
5:E:168:PHE:CE2	5:E:169:MET:HE2	2.38	0.58
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.84	0.58
2:B:157:VAL:HB	2:B:303:LEU:HD13	1.84	0.58
5:E:86:ASN:O	5:E:87:SER:CB	2.52	0.58
3:C:27:PRO:HG3	3:C:33:HIS:CD2	2.38	0.58
4:D:17:LEU:HG	10:D:323:HOH:O	2.03	0.58
5:E:74:TYR:OH	5:E:98:LEU:HD12	2.04	0.58
1:A:311:VAL:O	1:A:314:PRO:HD2	2.04	0.58
3:C:11:ILE:HG13	3:C:352:GLY:HA2	1.86	0.57
3:C:107:ASN:HD22	3:C:109:LYS:H	1.53	0.57
6:F:4:THR:HG23	6:F:55:ARG:NE	2.19	0.57
7:G:51:MET:HG3	7:G:87:LYS:HZ2	1.70	0.57
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.86	0.57
7:G:95:VAL:HG21	7:G:131:LYS:HB3	1.86	0.57
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.69	0.57
3:C:264:ASP:O	3:C:265:CYS:HB2	2.05	0.56
4:D:189:ARG:NH1	4:D:197:GLN:HB2	2.20	0.56
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.19	0.56
1:A:111:LEU:HD23	1:A:111:LEU:C	2.30	0.56
1:A:370:HIS:O	1:A:373:GLN:HG3	2.05	0.56
3:C:29:ASN:O	3:C:54:GLN:HA	2.05	0.56
3:C:252:PHE:HA	3:C:258:LEU:HD23	1.88	0.56
6:F:101:PHE:C	6:F:103:ILE:H	2.13	0.56
7:G:87:LYS:HD3	7:G:87:LYS:N	2.20	0.56
2:B:184:ILE:HD13	2:B:271:ILE:HD13	1.88	0.56
4:D:197:GLN:HE21	4:D:199:LEU:HD11	1.70	0.56
1:A:194:PRO:C	1:A:195:ILE:HD12	2.31	0.56
1:A:389:GLU:CD	1:A:414:PHE:HB2	2.31	0.56
4:D:19:PHE:HB3	4:D:106:LYS:HD3	1.87	0.56
2:B:174:SER:O	2:B:176:PRO:HD3	2.06	0.56
1:A:19:LEU:HD23	1:A:19:LEU:N	2.21	0.56
1:A:289:ASN:HD22	1:A:290:PRO:CD	2.18	0.56
3:C:50:GLU:OE1	3:C:88:PRO:HG3	2.06	0.56
5:E:95:MET:HG2	5:E:141:GLY:C	2.30	0.56
5:E:86:ASN:O	5:E:87:SER:HB3	2.06	0.56
1:A:257:THR:HG22	1:A:268:SER:CB	2.34	0.55
2:B:302:VAL:HA	2:B:345:GLU:CB	2.37	0.55
2:B:282:LEU:HD23	2:B:321:LEU:HD11	1.89	0.55
2:B:279:ALA:CB	2:B:320:GLU:HG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:20:ASP:OD1	7:G:22:ASN:HB2	2.05	0.55
5:E:169:MET:O	5:E:171:LYS:HG2	2.07	0.55
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.88	0.55
4:D:132:GLN:HE21	4:D:159:ASP:HA	1.72	0.55
3:C:184:PRO:HB2	3:C:231:ALA:CB	2.37	0.55
5:E:95:MET:HG2	5:E:141:GLY:CA	2.36	0.55
4:D:182:MET:HG3	4:D:200:PHE:CD1	2.42	0.54
1:A:309:ILE:HG23	1:A:310:ASP:H	1.72	0.54
3:C:96:ASN:O	3:C:97:ARG:HD3	2.07	0.54
2:B:158:ASP:HA	2:B:304:SER:O	2.08	0.54
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.38	0.54
2:B:287:GLN:NE2	2:B:298:TYR:OH	2.41	0.54
3:C:193:GLU:HB3	3:C:195:MET:HE2	1.88	0.54
2:B:163:VAL:HG22	2:B:164:THR:N	2.23	0.54
5:E:50:LYS:NZ	5:E:159:TRP:O	2.41	0.54
5:E:152:GLN:HB3	5:E:155:LYS:CE	2.38	0.54
2:B:180:ARG:HB2	2:B:281:LEU:HD21	1.88	0.54
2:B:184:ILE:HD13	2:B:271:ILE:CD1	2.38	0.53
3:C:155:VAL:HG11	3:C:180:PRO:HG2	1.90	0.53
6:F:53:ILE:N	6:F:53:ILE:HD12	2.22	0.53
1:A:19:LEU:HD13	1:A:96:VAL:HG13	1.89	0.53
3:C:257:SER:OG	3:C:372:VAL:N	2.37	0.53
2:B:330:LEU:C	2:B:332:GLY:H	2.16	0.53
5:E:105:ILE:HD13	5:E:130:ARG:NH1	2.23	0.53
3:C:170:SER:HB2	3:C:195:MET:HE3	1.89	0.53
3:C:358:ASP:OD1	3:C:360:ARG:HG2	2.09	0.53
1:A:395:HIS:HA	10:A:542:HOH:O	2.08	0.53
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.91	0.53
5:E:97:THR:O	5:E:101:THR:HG23	2.08	0.53
5:E:153:ASN:OD1	5:E:154:ASP:N	2.42	0.53
2:B:175:LEU:O	2:B:177:HIS:O	2.27	0.53
7:G:122:SER:O	7:G:126:LEU:HG	2.08	0.52
4:D:37:ASP:HB3	4:D:41:VAL:HB	1.91	0.52
4:D:263:HIS:HB3	4:D:267:ARG:NH1	2.24	0.52
7:G:51:MET:HB3	7:G:86:PHE:CE1	2.44	0.52
3:C:173:ILE:O	3:C:177:GLU:HG2	2.09	0.52
3:C:183:THR:HB	3:C:189:MET:HE1	1.92	0.52
1:A:183:GLY:HA3	1:A:413:VAL:HG21	1.91	0.52
1:A:223:THR:O	1:A:227:VAL:HG23	2.09	0.52
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.44	0.52
2:B:290:ASP:O	2:B:294:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:LEU:HD21	2:B:344:ILE:CG2	2.40	0.52
1:A:240:LYS:O	1:A:244:LYS:HG3	2.09	0.52
1:A:393:VAL:HG21	1:A:414:PHE:CE2	2.45	0.52
3:C:188:LYS:O	3:C:195:MET:HE1	2.10	0.52
6:F:145:GLU:O	6:F:149:MET:HG3	2.10	0.52
7:G:47:ARG:O	7:G:48:GLN:HG3	2.09	0.52
1:A:153:TRP:CE3	1:A:161:ARG:HD2	2.45	0.51
1:A:289:ASN:HD22	1:A:290:PRO:N	2.08	0.51
1:A:372:MET:HE2	1:A:379:PHE:CD1	2.46	0.51
1:A:67:ILE:HG22	1:A:68:GLU:HG2	1.93	0.51
4:D:205:PRO:HA	4:D:222:TYR:CD1	2.45	0.51
1:A:359:LYS:N	1:A:360:PRO:HD3	2.26	0.51
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.92	0.51
7:G:35:ALA:HB1	7:G:63:PRO:HA	1.91	0.51
7:G:140:SER:O	7:G:144:VAL:HG23	2.10	0.51
7:G:62:PRO:C	7:G:64:ILE:H	2.19	0.51
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.41	0.51
1:A:343:VAL:CG1	1:A:363:ILE:HD12	2.41	0.51
5:E:9:MET:SD	5:E:63:GLU:HG2	2.51	0.51
4:D:135:GLY:O	4:D:137:GLU:HG3	2.11	0.51
5:E:95:MET:HG2	5:E:141:GLY:HA3	1.92	0.51
1:A:172:ASP:OD2	1:A:198:ARG:NE	2.44	0.51
5:E:88:LYS:O	5:E:92:GLU:HG3	2.11	0.51
1:A:21:TYR:OH	1:A:103:ALA:HB2	2.11	0.50
5:E:5:HIS:HD2	5:E:65:ASP:OD2	1.93	0.50
1:A:18:LYS:HD2	1:A:18:LYS:N	2.26	0.50
2:B:290:ASP:HB2	2:B:293:THR:OG1	2.11	0.50
5:E:60:ILE:HD11	5:E:116:ILE:HG21	1.93	0.50
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.46	0.50
3:C:285:LEU:HB3	3:C:362:LEU:HD13	1.94	0.50
4:D:169:PHE:HB2	4:D:175:VAL:HG22	1.94	0.50
5:E:166:ARG:HG2	5:E:166:ARG:HH11	1.76	0.50
1:A:308:PRO:O	1:A:311:VAL:HG12	2.12	0.50
4:D:263:HIS:HB3	4:D:267:ARG:HH12	1.76	0.50
7:G:87:LYS:HE2	7:G:90:ASP:CG	2.37	0.50
1:A:68:GLU:O	1:A:69:LYS:C	2.55	0.49
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.94	0.49
4:D:111:HIS:CD2	4:D:115:MET:HE2	2.47	0.49
1:A:38:LYS:HD3	1:A:72:TYR:CE2	2.48	0.49
3:C:172:TYR:C	3:C:172:TYR:CD2	2.90	0.49
1:A:397:LYS:O	1:A:400:TYR:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:ILE:HG22	5:E:117:TYR:CD1	2.48	0.49
3:C:26:CYS:SG	3:C:55:VAL:HB	2.52	0.49
3:C:228:LEU:C	3:C:228:LEU:HD23	2.38	0.49
1:A:310:ASP:OD2	1:A:310:ASP:N	2.45	0.49
5:E:22:LEU:HD23	5:E:41:ILE:HD13	1.93	0.49
1:A:278:GLY:O	1:A:281:ILE:HG12	2.11	0.49
5:E:26:SER:HB2	5:E:139:GLU:HG2	1.95	0.49
3:C:234:LYS:O	3:C:235:MET:HB2	2.12	0.49
4:D:199:LEU:HB2	4:D:224:THR:HB	1.94	0.49
1:A:309:ILE:HG23	1:A:310:ASP:N	2.28	0.48
7:G:51:MET:HG3	7:G:87:LYS:HZ3	1.75	0.48
1:A:191:LYS:HB2	1:A:303:VAL:CG2	2.43	0.48
3:C:29:ASN:CB	3:C:31:GLU:H	2.23	0.48
4:D:64:TYR:CD2	4:D:92:ASN:HB3	2.48	0.48
4:D:212:THR:C	4:D:214:ALA:H	2.20	0.48
6:F:85:ILE:HD12	6:F:85:ILE:C	2.38	0.48
1:A:154:THR:HG22	1:A:370:HIS:HB2	1.94	0.48
6:F:158:ARG:O	6:F:162:GLU:HG3	2.14	0.48
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.79	0.48
3:C:107:ASN:ND2	3:C:107:ASN:C	2.61	0.48
4:D:206:PRO:HD3	4:D:222:TYR:CB	2.44	0.48
5:E:22:LEU:CD2	5:E:41:ILE:HD13	2.44	0.48
7:G:80:LEU:O	7:G:84:ILE:HD13	2.13	0.48
1:A:369:THR:HA	1:A:373:GLN:OE1	2.14	0.48
4:D:181:PHE:CE2	6:F:157:ALA:HA	2.49	0.48
7:G:99:ASP:O	7:G:102:GLY:N	2.41	0.48
3:C:7:LEU:HD12	3:C:9:GLU:HB2	1.96	0.48
3:C:157:LEU:O	3:C:168:ILE:HA	2.14	0.47
4:D:74:GLU:H	4:D:74:GLU:CD	2.22	0.47
5:E:95:MET:CG	5:E:141:GLY:HA3	2.44	0.47
1:A:339:LEU:HD23	1:A:365:VAL:CG1	2.44	0.47
3:C:126:GLU:CB	3:C:131:TRP:HZ3	2.25	0.47
3:C:179:ARG:HG3	3:C:179:ARG:NH1	2.26	0.47
4:D:75:LEU:HD23	4:D:75:LEU:C	2.39	0.47
5:E:56:LYS:HG3	5:E:170:ASN:HD21	1.80	0.47
6:F:163:GLU:O	6:F:167:ASN:ND2	2.47	0.47
4:D:118:ARG:HD3	4:D:118:ARG:C	2.40	0.47
7:G:52:THR:O	7:G:56:GLN:HG3	2.15	0.47
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.74	0.47
1:A:30:ILE:HD13	1:A:375:TYR:OH	2.14	0.47
5:E:9:MET:HE3	5:E:9:MET:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:5:LEU:HD13	6:F:55:ARG:NH1	2.29	0.47
7:G:87:LYS:HD3	7:G:87:LYS:H	1.80	0.47
3:C:13:CYS:SG	3:C:58:VAL:HG23	2.55	0.46
3:C:72:THR:HA	3:C:98:ALA:HB1	1.97	0.46
4:D:59:ILE:HB	4:D:116:LEU:HD13	1.97	0.46
5:E:95:MET:HA	5:E:95:MET:CE	2.44	0.46
5:E:152:GLN:HB3	5:E:155:LYS:HZ3	1.78	0.46
2:B:279:ALA:HB1	2:B:320:GLU:HG2	1.96	0.46
3:C:184:PRO:HB2	3:C:231:ALA:HB1	1.97	0.46
4:D:248:ARG:HD3	4:D:248:ARG:C	2.40	0.46
5:E:35:GLU:OE1	5:E:36:THR:N	2.48	0.46
2:B:254:VAL:HG12	2:B:258:ARG:HG3	1.98	0.46
3:C:212:ALA:HB3	3:C:255:GLU:OE2	2.16	0.46
3:C:370:LYS:O	3:C:371:ILE:CB	2.63	0.46
2:B:291:ILE:O	2:B:291:ILE:HG22	2.16	0.46
3:C:175:GLU:H	3:C:175:GLU:HG2	1.40	0.46
1:A:395:HIS:HB3	1:A:407:ILE:HD12	1.96	0.46
3:C:44:GLN:HE21	3:C:47:GLU:HG3	1.81	0.46
1:A:90:GLU:HG3	1:A:129:ILE:HG23	1.97	0.46
2:B:161:ASP:HB2	9:B:502:ATP:H5'1	1.97	0.46
4:D:169:PHE:HB2	4:D:175:VAL:CG2	2.46	0.45
1:A:153:TRP:CD2	1:A:161:ARG:HD2	2.52	0.45
4:D:228:PHE:H	4:D:231:HIS:CD2	2.31	0.45
4:D:53:THR:C	4:D:54:LYS:HD2	2.42	0.45
3:C:7:LEU:HD13	3:C:27:PRO:HB2	1.99	0.45
4:D:156:SER:O	4:D:157:LYS:HD2	2.17	0.45
4:D:182:MET:HG3	4:D:200:PHE:CE1	2.52	0.45
5:E:20:ALA:CB	5:E:22:LEU:HD13	2.45	0.45
1:A:152:SER:HB3	1:A:320:VAL:HG11	1.98	0.45
3:C:184:PRO:HB2	3:C:231:ALA:HB3	1.98	0.45
3:C:226:VAL:HG12	3:C:240:LEU:HB3	1.98	0.45
3:C:264:ASP:O	3:C:265:CYS:CB	2.64	0.45
5:E:24:ILE:CD1	5:E:135:GLN:HG2	2.47	0.45
4:D:95:LEU:HD11	4:D:116:LEU:HG	1.99	0.45
4:D:203:ARG:HA	4:D:217:GLY:O	2.17	0.45
5:E:150:ASP:OD2	5:E:152:GLN:HB2	2.17	0.45
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.47	0.45
2:B:330:LEU:O	2:B:332:GLY:N	2.50	0.45
3:C:144:THR:CB	6:F:28:GLN:HE21	2.30	0.45
3:C:327:ASN:HB2	3:C:351:ASP:HB3	1.99	0.45
7:G:51:MET:HB3	7:G:86:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:O	1:A:39:GLU:HB3	2.17	0.44
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.52	0.44
1:A:116:PRO:O	1:A:117:LEU:CB	2.64	0.44
2:B:257:GLU:HA	2:B:260:GLU:HB2	1.98	0.44
3:C:102:VAL:HG23	3:C:113:VAL:HG22	1.98	0.44
3:C:183:THR:CG2	3:C:184:PRO:N	2.81	0.44
7:G:114:PHE:CZ	7:G:126:LEU:HD23	2.52	0.44
3:C:207:GLY:O	3:C:219:TRP:HA	2.18	0.44
4:D:136:LYS:HE3	4:D:136:LYS:HB2	1.83	0.44
3:C:61:ALA:HB1	3:C:108:GLU:OE1	2.17	0.44
6:F:105:ARG:HG2	6:F:105:ARG:HH11	1.83	0.44
4:D:159:ASP:OD2	4:D:159:ASP:N	2.48	0.44
4:D:197:GLN:HE21	4:D:199:LEU:CD1	2.31	0.44
6:F:2:THR:HG23	6:F:3:ALA:N	2.29	0.44
1:A:129:ILE:O	1:A:133:SER:HB2	2.18	0.44
3:C:119:VAL:HG22	3:C:120:ILE:N	2.33	0.44
4:D:199:LEU:N	4:D:199:LEU:HD12	2.33	0.44
5:E:28:PHE:HE1	5:E:142:LEU:HD22	1.82	0.44
1:A:172:ASP:CG	1:A:198:ARG:HG3	2.42	0.44
2:B:318:GLU:CG	2:B:344:ILE:HD12	2.46	0.44
4:D:223:ILE:HD12	4:D:223:ILE:N	2.32	0.44
4:D:182:MET:HE3	4:D:182:MET:HA	2.00	0.43
2:B:299:LYS:O	2:B:300:HIS:ND1	2.51	0.43
3:C:60:TRP:HE1	3:C:65:ASN:ND2	2.16	0.43
5:E:142:LEU:O	5:E:145:CYS:HB2	2.18	0.43
1:A:369:THR:HG23	10:A:527:HOH:O	2.18	0.43
2:B:257:GLU:H	2:B:257:GLU:CD	2.25	0.43
2:B:280:GLU:HA	2:B:324:LEU:HD11	2.00	0.43
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.53	0.43
3:C:13:CYS:HA	3:C:331:GLN:NE2	2.33	0.43
1:A:151:ALA:O	1:A:154:THR:HB	2.18	0.43
5:E:16:ILE:O	5:E:16:ILE:CG2	2.66	0.43
6:F:53:ILE:HA	7:G:114:PHE:CD1	2.53	0.43
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.54	0.43
4:D:32:GLU:OE2	4:D:44:HIS:NE2	2.51	0.43
5:E:32:ALA:HA	5:E:33:PRO:HD3	1.89	0.43
1:A:217:PRO:C	1:A:219:GLN:H	2.26	0.43
3:C:21:THR:HG22	3:C:22:GLN:CG	2.48	0.43
3:C:178:GLU:O	3:C:179:ARG:C	2.61	0.43
5:E:74:TYR:CE2	5:E:137:ARG:HA	2.54	0.43
5:E:132:TYR:O	5:E:135:GLN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:8:TYR:CG	6:F:55:ARG:HB2	2.54	0.43
7:G:37:PRO:HG3	7:G:58:ALA:O	2.18	0.43
3:C:33:HIS:HD2	10:C:395:HOH:O	2.02	0.43
3:C:183:THR:CG2	3:C:185:TRP:H	2.12	0.43
4:D:189:ARG:NH2	4:D:197:GLN:HG3	2.33	0.43
4:D:64:TYR:HB3	4:D:92:ASN:ND2	2.33	0.43
4:D:77:LYS:HD2	4:D:77:LYS:HA	1.76	0.43
6:F:2:THR:O	6:F:3:ALA:HB3	2.19	0.43
1:A:156:ARG:CB	1:A:368:ILE:HG23	2.48	0.42
1:A:226:ALA:O	1:A:230:ARG:HD3	2.19	0.42
2:B:223:VAL:HG23	2:B:310:TYR:CB	2.49	0.42
4:D:258:SER:O	4:D:262:ILE:HG12	2.19	0.42
6:F:76:VAL:HG12	6:F:77:LYS:N	2.34	0.42
2:B:159:SER:HB2	2:B:164:THR:HG23	2.02	0.42
2:B:281:LEU:O	2:B:281:LEU:HD23	2.19	0.42
2:B:222:TYR:O	2:B:259:PHE:HA	2.19	0.42
3:C:44:GLN:NE2	3:C:47:GLU:HG3	2.34	0.42
3:C:283:GLY:O	3:C:284:ARG:HB2	2.19	0.42
5:E:10:ASP:HB3	5:E:12:ASP:OD1	2.20	0.42
5:E:24:ILE:O	5:E:24:ILE:HG13	2.19	0.42
1:A:152:SER:O	1:A:154:THR:N	2.51	0.42
1:A:343:VAL:HG11	1:A:363:ILE:HB	2.00	0.42
3:C:142:ARG:HG3	3:C:142:ARG:NH1	2.33	0.42
5:E:85:CYS:HB2	5:E:90:GLN:CD	2.45	0.42
1:A:19:LEU:HD23	1:A:19:LEU:H	1.84	0.42
1:A:61:PHE:C	1:A:66:ALA:HB2	2.45	0.42
1:A:91:ARG:O	1:A:94:GLU:HB2	2.20	0.42
2:B:318:GLU:O	2:B:322:LYS:HG3	2.20	0.42
3:C:189:MET:HA	3:C:195:MET:CE	2.49	0.42
3:C:228:LEU:HD23	3:C:229:ALA:N	2.34	0.42
3:C:268:VAL:HA	3:C:284:ARG:H	1.85	0.42
4:D:141:ARG:NH2	4:D:212:THR:CG2	2.82	0.42
4:D:263:HIS:CD2	4:D:266:MET:HE2	2.53	0.42
4:D:269:LYS:HD2	4:D:269:LYS:HA	1.85	0.42
5:E:87:SER:N	5:E:154:ASP:HA	2.33	0.42
7:G:74:ARG:O	7:G:78:ILE:HG13	2.20	0.42
1:A:328:PHE:CE1	9:A:501:ATP:H2	2.37	0.42
3:C:226:VAL:CG1	3:C:240:LEU:HB3	2.49	0.42
4:D:132:GLN:HB2	4:D:156:SER:OG	2.19	0.42
1:A:282:PHE:CD2	1:A:331:PHE:HE1	2.38	0.42
3:C:153:ASN:OD1	3:C:153:ASN:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:THR:CG2	6:F:3:ALA:H	2.22	0.42
6:F:4:THR:C	6:F:7:PRO:HD2	2.45	0.42
6:F:130:LYS:HA	6:F:130:LYS:CE	2.42	0.42
7:G:87:LYS:O	7:G:88:ALA:C	2.62	0.42
1:A:247:THR:HG22	1:A:248:ASP:N	2.35	0.42
1:A:248:ASP:OD2	1:A:251:LYS:HD3	2.20	0.42
2:B:167:CYS:HA	2:B:168:PRO:HD3	1.88	0.42
3:C:156:LEU:HD21	3:C:189:MET:HE2	2.00	0.42
3:C:193:GLU:CG	3:C:195:MET:HE2	2.49	0.42
6:F:73:SER:HB3	6:F:112:TYR:CG	2.55	0.42
2:B:184:ILE:HG13	2:B:265:LEU:HD23	2.01	0.41
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.50	0.41
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.20	0.41
4:D:6:VAL:HG21	4:D:242:ASN:HB3	2.02	0.41
5:E:134:GLN:O	5:E:138:GLN:HG2	2.20	0.41
3:C:102:VAL:HA	3:C:112:ALA:O	2.20	0.41
4:D:146:TYR:OH	4:D:248:ARG:HG3	2.19	0.41
4:D:269:LYS:O	4:D:272:ASP:HB2	2.21	0.41
5:E:152:GLN:O	5:E:153:ASN:O	2.39	0.41
3:C:183:THR:HB	3:C:189:MET:CE	2.50	0.41
5:E:60:ILE:CD1	5:E:116:ILE:HG23	2.51	0.41
5:E:82:LEU:HD12	5:E:82:LEU:HA	1.88	0.41
5:E:145:CYS:O	5:E:149:PHE:HD1	2.03	0.41
1:A:289:ASN:HD22	1:A:289:ASN:C	2.28	0.41
4:D:188:GLY:HA3	6:F:165:LEU:HD23	2.03	0.41
6:F:2:THR:C	6:F:4:THR:N	2.77	0.41
7:G:93:LYS:NZ	7:G:93:LYS:HB3	2.36	0.41
1:A:168:ILE:HD13	1:A:335:LEU:HD11	2.02	0.41
2:B:254:VAL:HG13	2:B:257:GLU:HG2	2.03	0.41
5:E:62:ASN:C	5:E:64:ALA:N	2.73	0.41
3:C:366:LEU:HD12	3:C:366:LEU:N	2.35	0.41
4:D:186:LYS:NZ	4:D:200:PHE:H	2.19	0.41
5:E:166:ARG:HG2	5:E:166:ARG:NH1	2.36	0.41
6:F:20:LEU:HD23	6:F:20:LEU:HA	1.92	0.41
1:A:87:ASP:OD2	4:D:267:ARG:HD2	2.21	0.41
1:A:289:ASN:HA	1:A:290:PRO:HD3	1.92	0.41
1:A:289:ASN:ND2	1:A:291:ASP:H	2.18	0.41
2:B:319:ARG:O	2:B:323:GLN:HG3	2.21	0.41
1:A:328:PHE:CZ	9:A:501:ATP:H2	2.38	0.41
2:B:166:ILE:HD12	2:B:281:LEU:HD23	2.02	0.41
3:C:167:ARG:HG2	3:C:197:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:PHE:CE1	3:C:258:LEU:HD21	2.56	0.41
3:C:358:ASP:HB3	3:C:361:SER:HB2	2.01	0.41
4:D:30:ALA:HA	4:D:52:LYS:HG2	2.03	0.41
4:D:44:HIS:ND1	4:D:88:GLU:OE2	2.49	0.41
6:F:2:THR:OG1	6:F:3:ALA:N	2.50	0.41
6:F:114:ILE:HG13	6:F:115:SER:N	2.36	0.41
5:E:30:GLY:HA3	5:E:135:GLN:CD	2.46	0.41
5:E:152:GLN:CB	5:E:155:LYS:HD2	2.51	0.41
5:E:153:ASN:CG	5:E:154:ASP:N	2.79	0.41
7:G:41:GLU:O	7:G:44:SER:HB3	2.20	0.41
1:A:260:ASN:HB3	1:A:262:ILE:O	2.20	0.40
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.80	0.40
6:F:20:LEU:HD23	6:F:70:VAL:CG2	2.45	0.40
7:G:75:ALA:O	7:G:79:VAL:HG23	2.21	0.40
2:B:163:VAL:CG2	2:B:164:THR:N	2.84	0.40
2:B:223:VAL:HG23	2:B:310:TYR:HB3	2.04	0.40
2:B:326:LEU:O	2:B:326:LEU:HG	2.20	0.40
5:E:130:ARG:HH11	5:E:130:ARG:HB2	1.86	0.40
1:A:374:ARG:HG2	1:A:375:TYR:CE2	2.56	0.40
2:B:161:ASP:OD2	9:B:502:ATP:H3'	2.21	0.40
3:C:32:VAL:HB	3:C:48:LEU:HB2	2.03	0.40
5:E:96:TYR:O	5:E:100:ILE:HG12	2.21	0.40
1:A:262:ILE:HG22	1:A:263:SER:N	2.36	0.40
3:C:183:THR:HG21	3:C:185:TRP:HD1	1.87	0.40
5:E:87:SER:HA	5:E:153:ASN:OD1	2.21	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	389/418 (93%)	356 (92%)	29 (8%)	4 (1%)	12 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	195/394 (50%)	175 (90%)	14 (7%)	6 (3%)	3	7
3	C	337/372 (91%)	315 (94%)	18 (5%)	4 (1%)	10	24
4	D	276/300 (92%)	260 (94%)	15 (5%)	1 (0%)	30	51
5	E	171/178 (96%)	158 (92%)	9 (5%)	4 (2%)	5	11
6	F	165/168 (98%)	155 (94%)	8 (5%)	2 (1%)	10	24
7	G	131/151 (87%)	113 (86%)	13 (10%)	5 (4%)	2	5
All	All	1664/1981 (84%)	1532 (92%)	106 (6%)	26 (2%)	7	18

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	SER
2	B	171	GLU
2	B	345	GLU
3	C	371	ILE
5	E	87	SER
5	E	153	ASN
6	F	102	PHE
3	C	203	GLY
7	G	37	PRO
1	A	69	LYS
1	A	263	SER
2	B	331	LYS
3	C	179	ARG
7	G	48	GLN
2	B	278	VAL
2	B	348	PRO
3	C	284	ARG
4	D	136	LYS
7	G	88	ALA
7	G	100	LYS
5	E	49	PHE
5	E	151	PRO
6	F	56	ASN
1	A	194	PRO
2	B	329	VAL
7	G	63	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	333/363 (92%)	319 (96%)	14 (4%)	26	52
2	B	151/345 (44%)	141 (93%)	10 (7%)	15	33
3	C	288/313 (92%)	276 (96%)	12 (4%)	26	52
4	D	242/264 (92%)	238 (98%)	4 (2%)	53	77
5	E	156/159 (98%)	146 (94%)	10 (6%)	16	35
6	F	154/155 (99%)	148 (96%)	6 (4%)	28	54
7	G	111/124 (90%)	106 (96%)	5 (4%)	24	49
All	All	1435/1723 (83%)	1374 (96%)	61 (4%)	26	51

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	67	ILE
1	A	71	THR
1	A	88	LEU
1	A	143	VAL
1	A	154	THR
1	A	155	SER
1	A	172	ASP
1	A	191	LYS
1	A	230	ARG
1	A	239	VAL
1	A	255	GLN
1	A	310	ASP
1	A	335	LEU
2	B	175	LEU
2	B	182	LEU
2	B	184	ILE
2	B	200	ARG
2	B	220	LEU
2	B	231	GLN

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Mol	Chain	Res	Type
2	B	237	THR
2	B	257	GLU
2	B	274	GLU
2	B	320	GLU
3	C	9	GLU
3	C	21	THR
3	C	90	LEU
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	175	GLU
3	C	179	ARG
3	C	183	THR
3	C	202	CYS
3	C	321	LEU
3	C	368	ASP
4	D	33	VAL
4	D	116	LEU
4	D	171	ASP
4	D	265	ARG
5	E	9	MET
5	E	22	LEU
5	E	38	ASP
5	E	63	GLU
5	E	82	LEU
5	E	95	MET
5	E	98	LEU
5	E	130	ARG
5	E	145	CYS
5	E	146	GLU
6	F	2	THR
6	F	31	GLU
6	F	57	GLU
6	F	102	PHE
6	F	104	LEU
6	F	165	LEU
7	G	18	GLU
7	G	21	GLU
7	G	27	GLU
7	G	64	ILE
7	G	93	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	122	ASN
1	A	144	GLN
1	A	205	GLN
1	A	206	GLN
1	A	243	ASN
1	A	255	GLN
1	A	289	ASN
1	A	318	ASN
1	A	370	HIS
1	A	395	HIS
1	A	411	ASN
2	B	205	ASN
2	B	267	GLN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	22	GLN
3	C	44	GLN
3	C	46	HIS
3	C	65	ASN
3	C	107	ASN
3	C	331	GLN
4	D	101	ASN
4	D	132	GLN
4	D	140	ASN
4	D	197	GLN
4	D	231	HIS
6	F	28	GLN
6	F	49	GLN
6	F	78	GLN
6	F	120	ASN
6	F	125	GLN
6	F	137	HIS
6	F	167	ASN
7	G	61	ASN
7	G	65	ASN
7	G	69	GLN
7	G	96	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ATP	B	502	-	32,33,33	1.60	8 (25%)	48,52,52	1.71	9 (18%)
9	ATP	A	501	8	32,33,33	1.53	5 (15%)	48,52,52	1.70	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ATP	B	502	-	-	1/22/38/38	0/3/3/3
9	ATP	A	501	8	-	2/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	ATP	C2-N1	3.89	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	501	ATP	C2-N1	3.77	1.40	1.33
9	B	502	ATP	PG-O1G	3.65	1.61	1.50
9	A	501	ATP	PG-O1G	3.54	1.61	1.50
9	B	502	ATP	C5-N7	-3.13	1.33	1.39
9	A	501	ATP	C5-N7	-3.08	1.33	1.39
9	B	502	ATP	C8-N9	-2.43	1.33	1.37
9	A	501	ATP	C8-N9	-2.30	1.33	1.37
9	B	502	ATP	C4-N9	-2.21	1.33	1.37
9	B	502	ATP	PB-O3B	2.10	1.61	1.59
9	B	502	ATP	PB-O3A	2.07	1.61	1.59
9	B	502	ATP	PA-O3A	2.07	1.61	1.59
9	A	501	ATP	C4-N9	-2.04	1.33	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	502	ATP	N3-C2-N1	-5.55	120.19	128.58
9	A	501	ATP	N3-C2-N1	-5.53	120.21	128.58
9	B	502	ATP	C5-C4-N3	-4.47	120.56	126.72
9	B	502	ATP	C2-N3-C4	4.20	122.09	111.83
9	A	501	ATP	C2-N3-C4	4.05	121.72	111.83
9	A	501	ATP	C5-C4-N3	-4.03	121.16	126.72
9	A	501	ATP	N9-C8-N7	-3.09	109.55	113.94
9	B	502	ATP	N3-C4-N9	3.06	132.36	127.17
9	B	502	ATP	N9-C8-N7	-2.98	109.71	113.94
9	A	501	ATP	N3-C4-N9	2.83	131.97	127.17
9	A	501	ATP	C5-N7-C8	2.74	107.76	103.45
9	B	502	ATP	C4-C5-N7	-2.65	107.55	110.58
9	A	501	ATP	O3G-PG-O3B	2.63	113.47	104.64
9	B	502	ATP	C5-N7-C8	2.62	107.57	103.45
9	A	501	ATP	C4-C5-N7	-2.61	107.60	110.58
9	B	502	ATP	O3G-PG-O3B	2.50	113.02	104.64
9	A	501	ATP	C4-N9-C8	2.37	108.22	105.74
9	B	502	ATP	C4-N9-C8	2.24	108.09	105.74
9	A	501	ATP	O4'-C1'-C2'	-2.10	102.13	106.62

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	501	ATP	PG-O3B-PB-O1B
9	A	501	ATP	PG-O3B-PB-O2B

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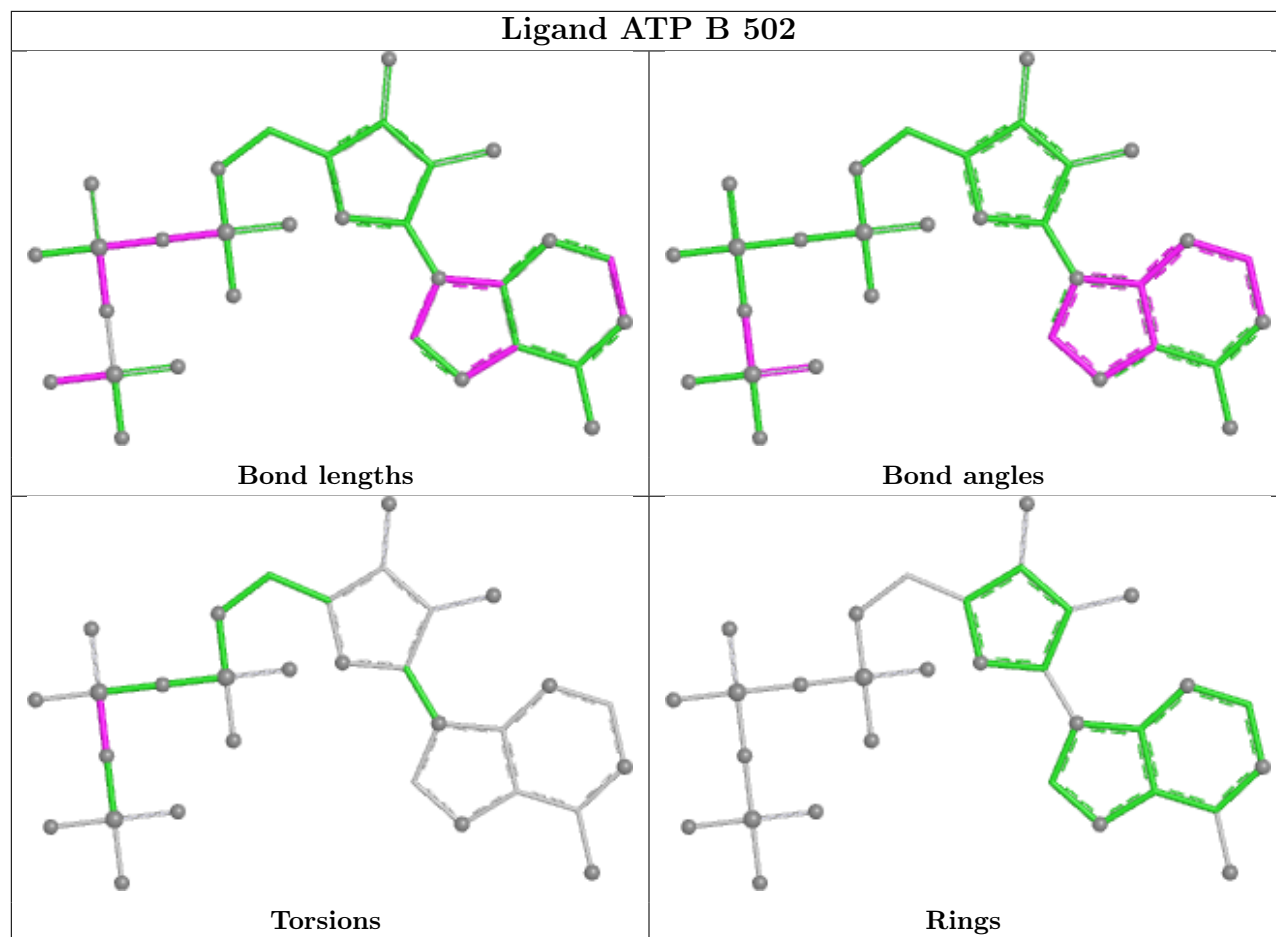
Mol	Chain	Res	Type	Atoms
9	B	502	ATP	PG-O3B-PB-O2B

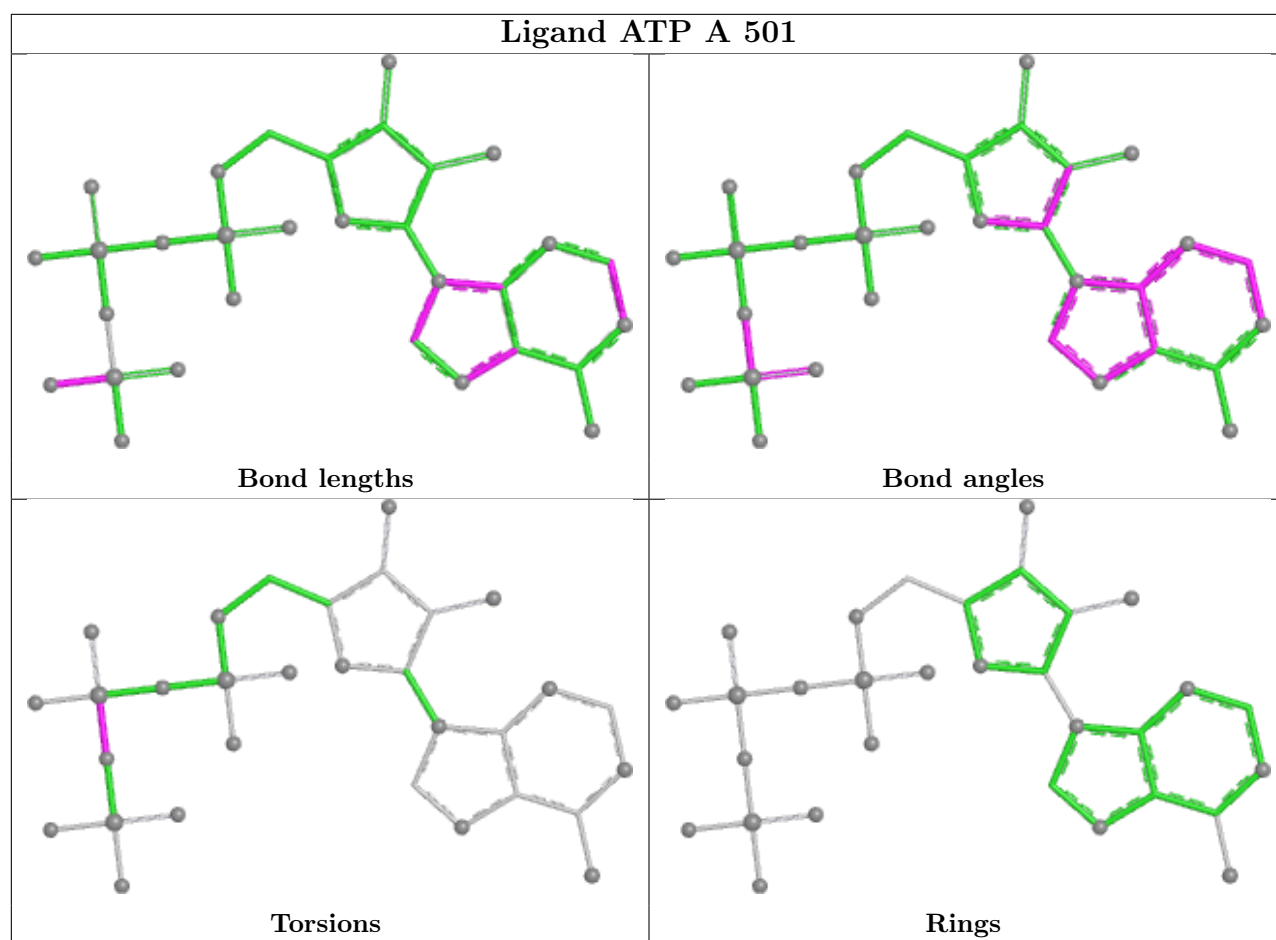
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	502	ATP	3	0
9	A	501	ATP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	397/418 (94%)	0.03	23 (5%) 29 25	25, 48, 81, 96	0
2	B	197/394 (50%)	0.65	25 (12%) 8 6	34, 62, 96, 111	0
3	C	341/372 (91%)	-0.17	6 (1%) 67 65	27, 41, 69, 92	0
4	D	280/300 (93%)	-0.08	6 (2%) 63 60	27, 44, 78, 87	0
5	E	173/178 (97%)	0.33	6 (3%) 47 42	37, 58, 85, 100	0
6	F	167/168 (99%)	-0.22	2 (1%) 76 74	30, 43, 59, 89	0
7	G	135/151 (89%)	0.79	16 (11%) 9 7	35, 72, 96, 103	0
All	All	1690/1981 (85%)	0.11	84 (4%) 34 30	25, 49, 88, 111	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	208	GLU	5.9
1	A	354	SER	4.5
2	B	291	ILE	4.3
1	A	156	ARG	4.1
3	C	127	GLN	3.9
1	A	159	GLY	3.9
5	E	35	GLU	3.8
2	B	349	ARG	3.8
7	G	149	LYS	3.7
2	B	153	THR	3.6
2	B	342	ILE	3.6
7	G	28	ASP	3.6
1	A	68	GLU	3.5
7	G	50	ASN	3.4
1	A	51	VAL	3.4
2	B	343	ARG	3.4
2	B	276	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	329	VAL	3.1
4	D	216	VAL	3.1
1	A	415	GLY	3.0
1	A	192	HIS	3.0
1	A	52	MET	3.0
2	B	171	GLU	2.9
1	A	261	ALA	2.9
2	B	302	VAL	2.9
2	B	334	VAL	2.9
7	G	25	VAL	2.9
2	B	154	GLY	2.8
4	D	213	ASP	2.8
6	F	2	THR	2.7
7	G	19	TYR	2.7
1	A	262	ILE	2.7
1	A	352	GLU	2.7
2	B	335	GLU	2.7
7	G	46	LEU	2.7
7	G	35	ALA	2.7
2	B	170	TYR	2.6
1	A	259	ILE	2.6
7	G	27	GLU	2.6
3	C	319	ALA	2.6
3	C	372	VAL	2.6
7	G	119	ASP	2.5
7	G	16	VAL	2.5
1	A	2	ALA	2.5
1	A	361	LYS	2.5
5	E	36	THR	2.5
5	E	154	ASP	2.5
3	C	75	ASN	2.4
5	E	155	LYS	2.4
5	E	151	PRO	2.4
4	D	215	ALA	2.4
4	D	211	ASP	2.3
4	D	206	PRO	2.3
7	G	47	ARG	2.3
1	A	155	SER	2.3
2	B	337	LEU	2.3
7	G	23	LYS	2.3
7	G	120	ASN	2.3
2	B	182	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	341	LYS	2.3
3	C	129	ASN	2.3
2	B	340	PHE	2.2
1	A	71	THR	2.2
2	B	348	PRO	2.2
1	A	268	SER	2.2
1	A	414	PHE	2.2
6	F	3	ALA	2.2
2	B	274	GLU	2.2
2	B	178	LEU	2.2
1	A	351	GLU	2.1
7	G	74	ARG	2.1
3	C	202	CYS	2.1
2	B	328	ARG	2.1
2	B	333	ASP	2.1
1	A	161	ARG	2.1
1	A	265	LYS	2.1
5	E	84	LYS	2.1
7	G	66	THR	2.1
1	A	353	LEU	2.1
2	B	298	TYR	2.1
2	B	294	ARG	2.0
7	G	21	GLU	2.0
2	B	177	HIS	2.0
1	A	374	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

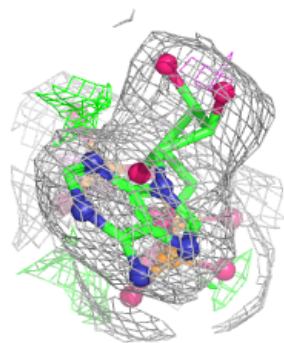
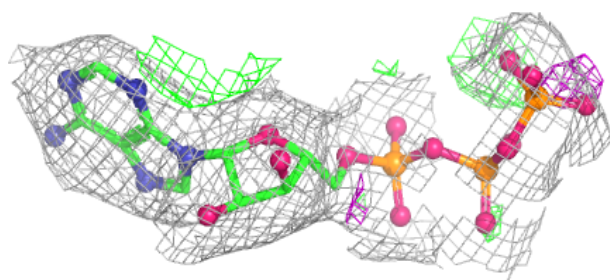
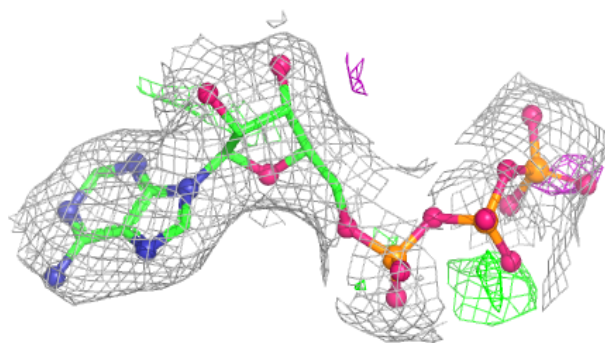
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

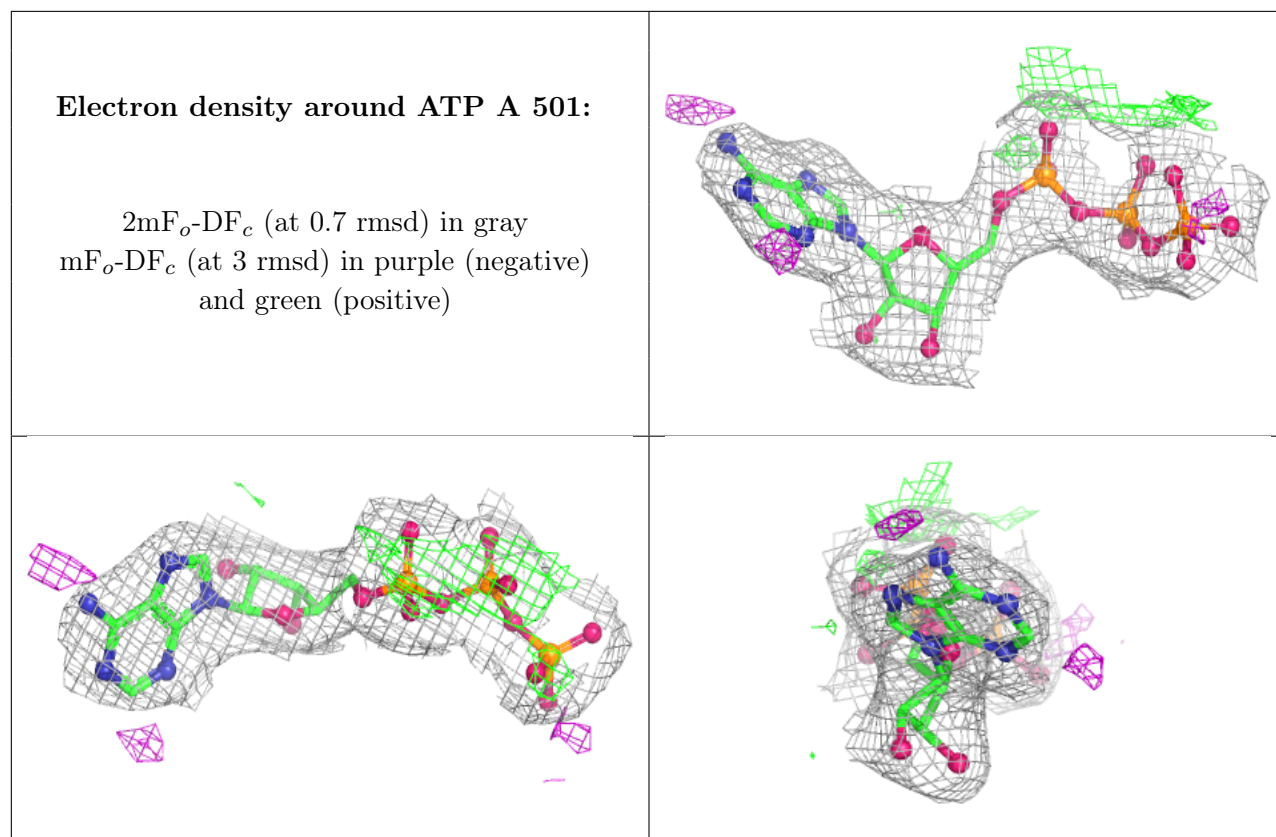
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	ATP	B	502	31/31	0.89	0.09	51,58,88,89	0
8	MG	A	500	1/1	0.94	0.21	43,43,43,43	0
9	ATP	A	501	31/31	0.96	0.07	41,45,48,51	0

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 502:

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 ⓘ

There are no such residues in this entry.