



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2021 – 12:30 PM EDT

PDB ID : 7KRW
Title : Stimulating state of near full-length Hsp70 DnaK fused with a substrate peptide
Authors : Wang, W.; Hendrickson, W.A.
Deposited on : 2020-11-20
Resolution : 7.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

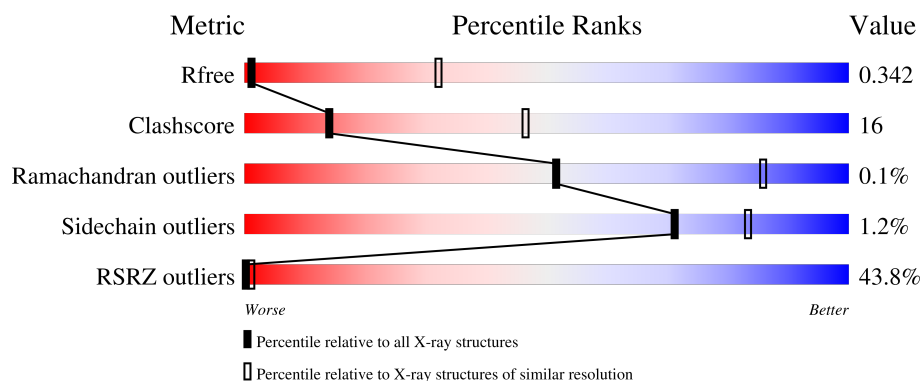
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	622	<div> <div>43%</div> <div>70% 27% ..</div> </div>
1	B	622	<div> <div>39%</div> <div>60% 27% 13%</div> </div>
1	C	622	<div> <div>37%</div> <div>57% 29% 13%</div> </div>
1	D	622	<div> <div>38%</div> <div>59% 27% 13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17034 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.

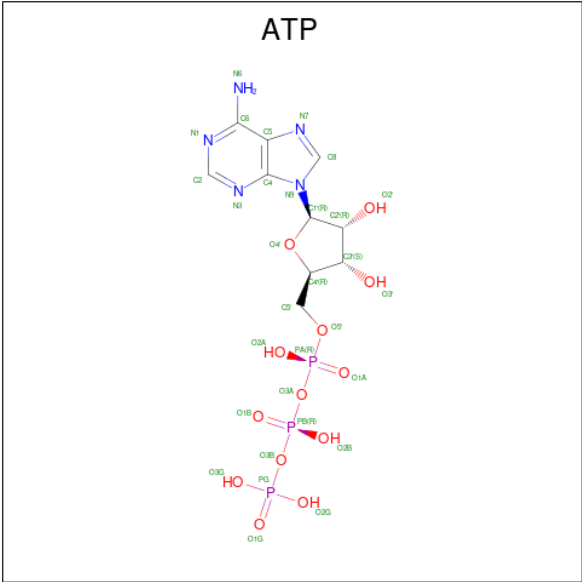
- Molecule 1 is a protein called Chaperone protein DnaK fused with substrate peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	541	Total	C	N	O	S	0	0	0
			4105	2557	712	823	13			
1	B	541	Total	C	N	O	S	0	0	0
			4105	2557	712	823	13			
1	A	608	Total	C	N	O	S	0	0	0
			4595	2857	799	924	15			
1	D	541	Total	C	N	O	S	0	0	0
			4105	2557	712	823	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	199	ALA	THR	engineered mutation	UNP A0A6D2W465
B	199	ALA	THR	engineered mutation	UNP A0A6D2W465
A	199	ALA	THR	engineered mutation	UNP A0A6D2W465
D	199	ALA	THR	engineered mutation	UNP A0A6D2W465

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

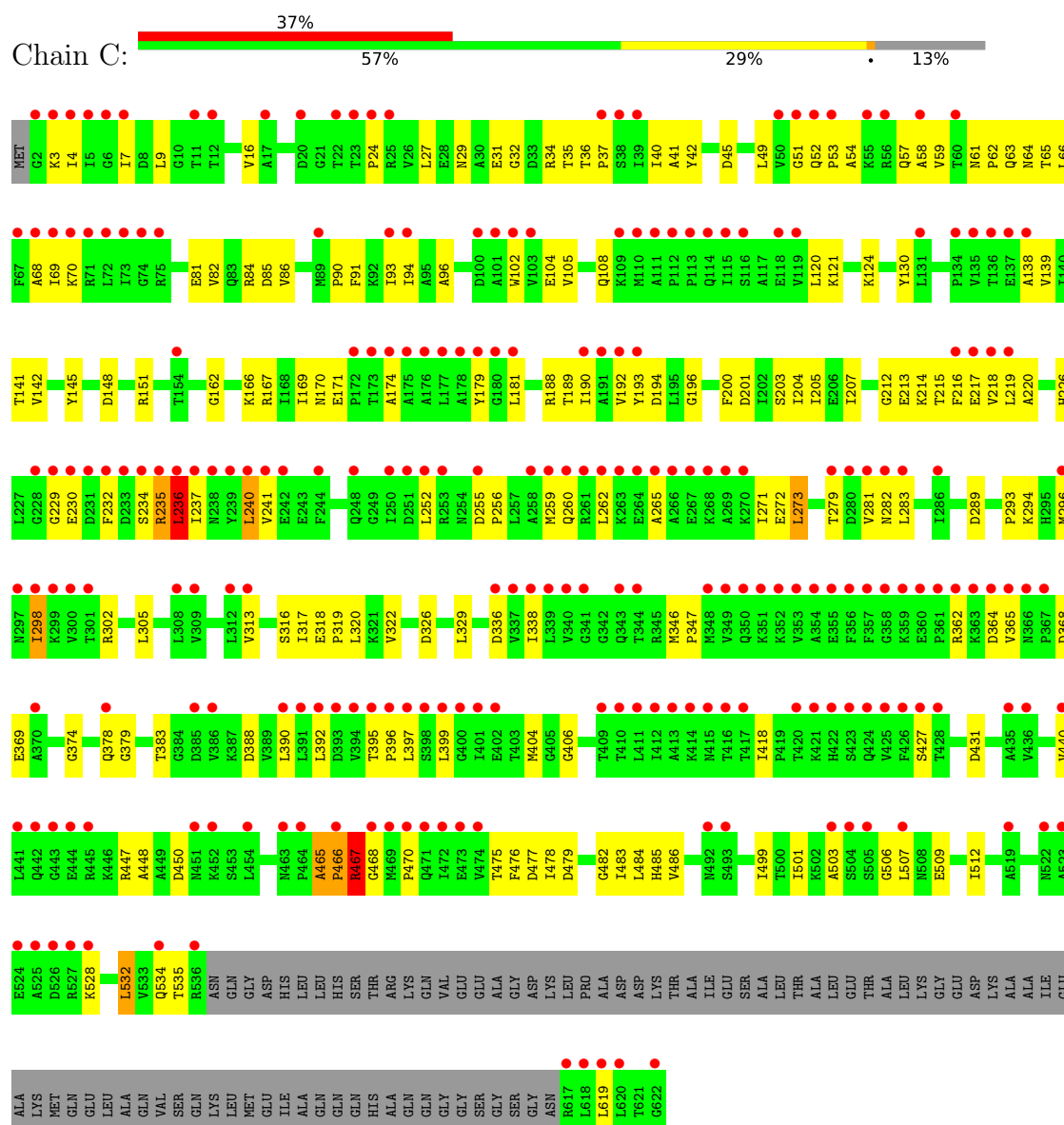


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

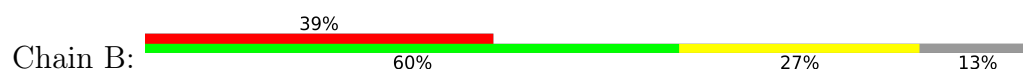
3 Residue-property plots

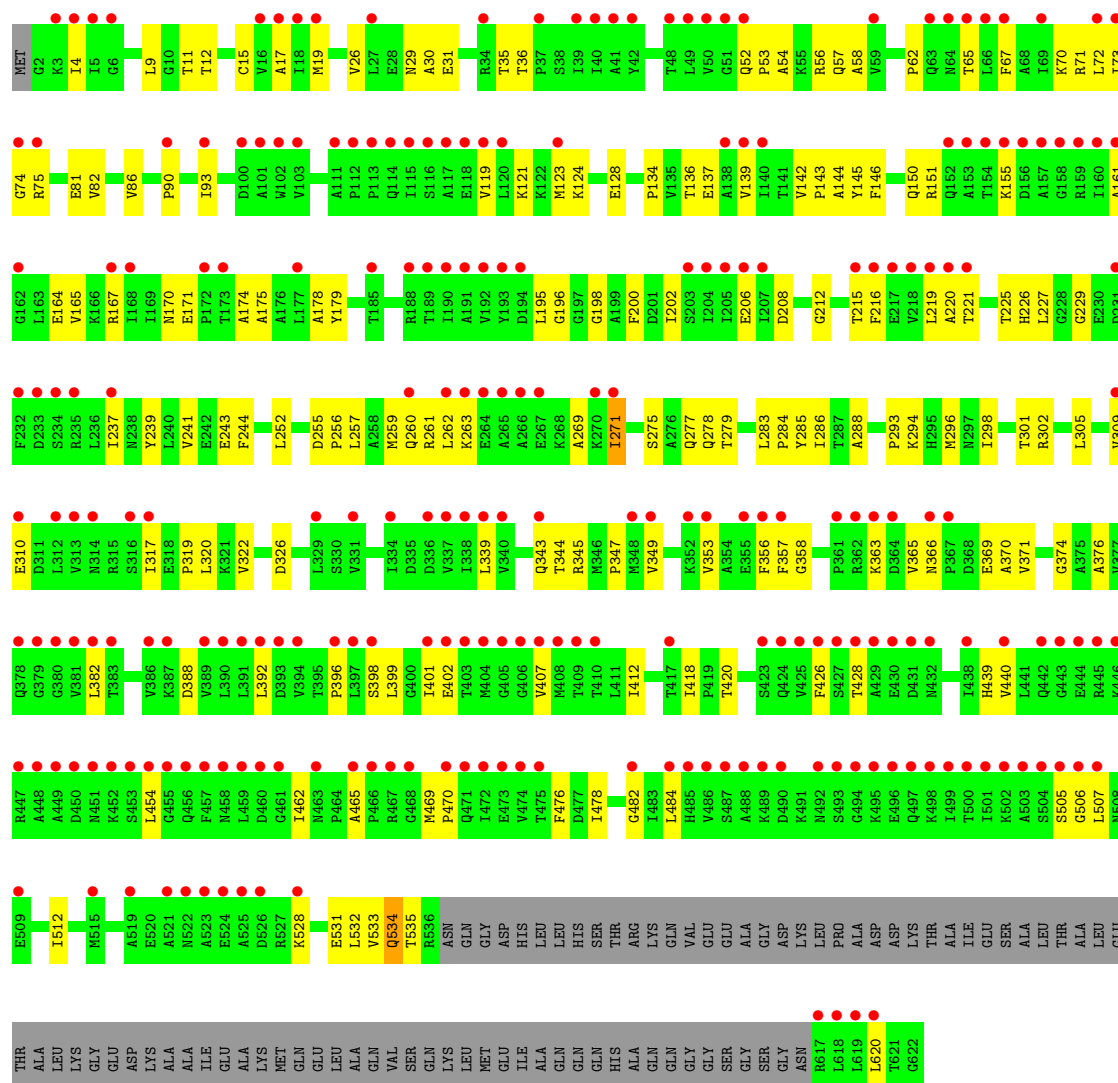
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

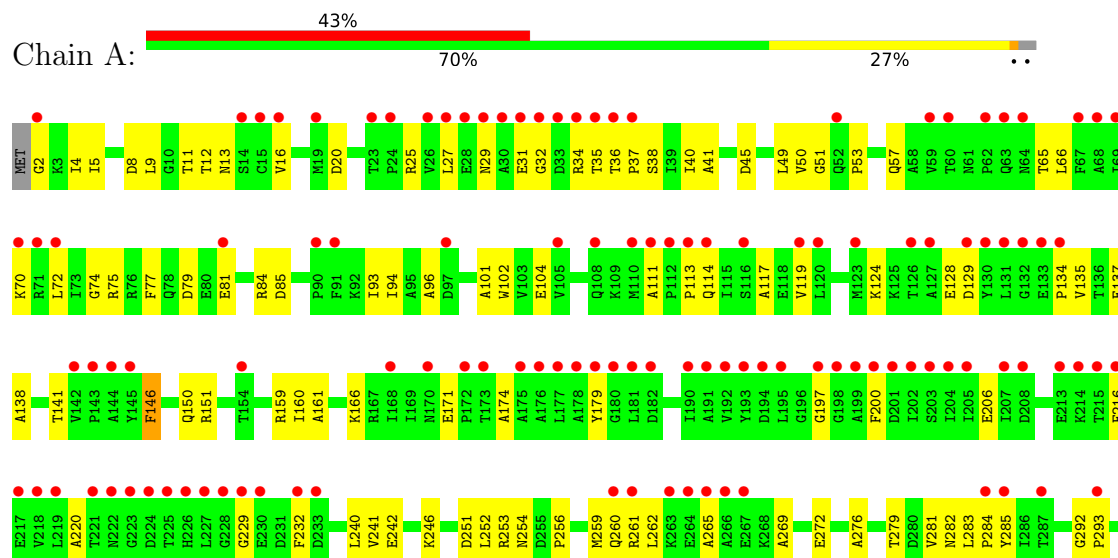


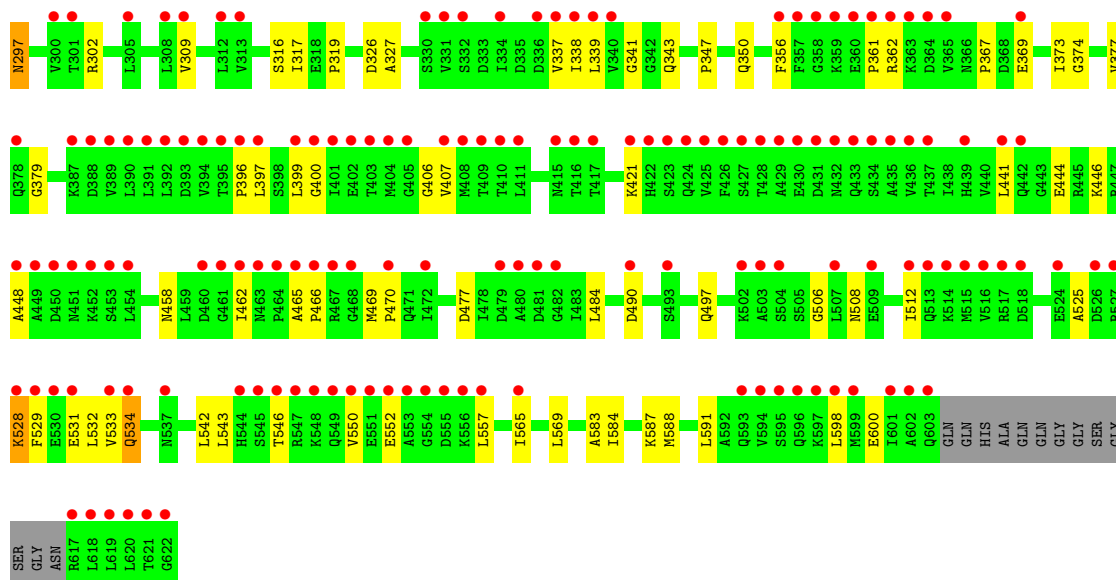
- Molecule 1: Chaperone protein DnaK fused with substrate peptide



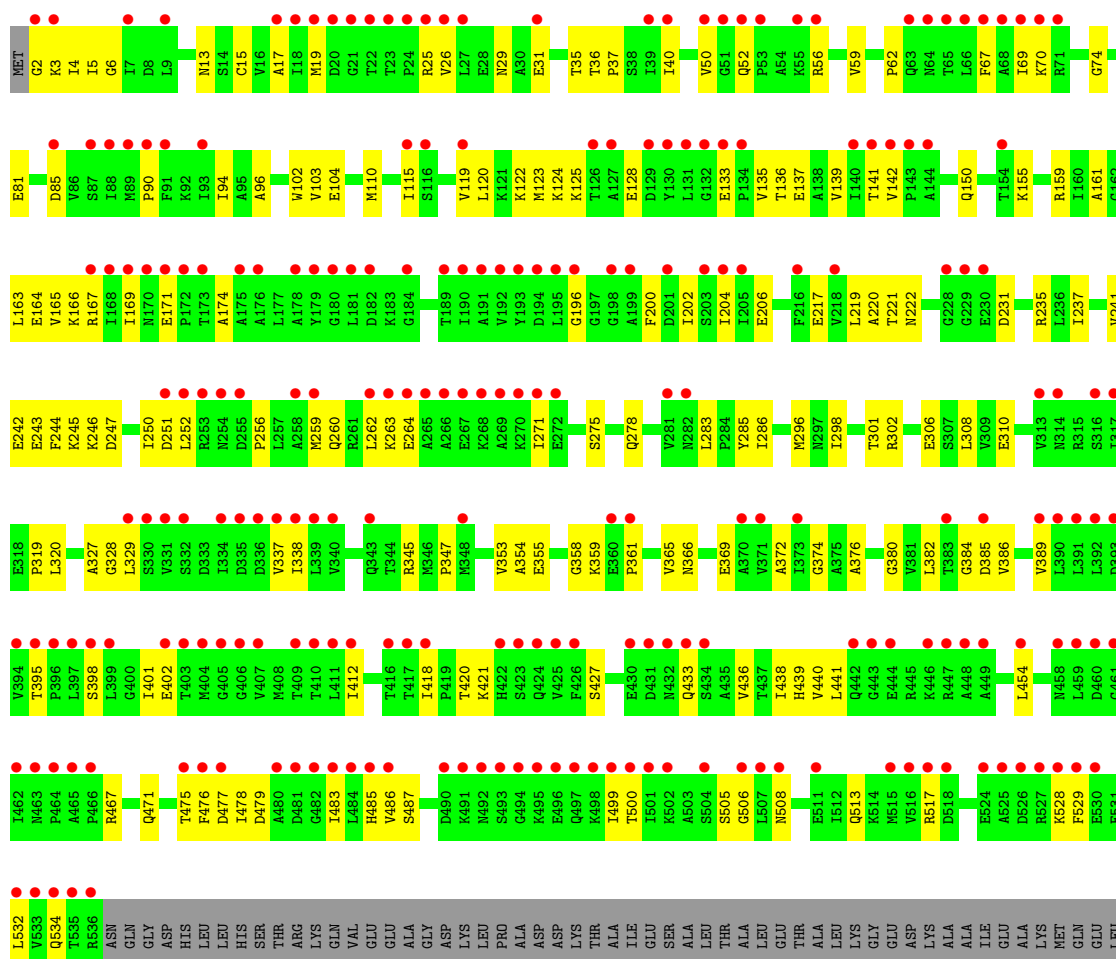
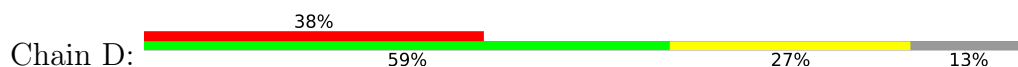


• Molecule 1: Chaperone protein DnaK fused with substrate peptide





• Molecule 1: Chaperone protein DnaK fused with substrate peptide



ALA	GLN	VAL	SER	GLN	LYS	LEU	MET	GLU	ILE	ALA	GLN	GLN	GLN	HIS	ALA	GLN	GLN	GLY	GLY	SER	GLY	SER	GLY	ASN	R617	L618	L619	L620	T621	G622

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	294.20Å 294.20Å 294.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.63 – 7.70 38.63 – 7.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.63-7.70) 94.6 (38.63-7.70)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 7.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.304 , 0.316 0.300 , 0.342	Depositor DCC
R_{free} test set	258 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	453.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 500.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.309 for -l,-k,-h	Xtriage
Reported twinning fraction	0.430 for -l,-k,-h	Depositor
Outliers	0 of 5015 reflections	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	17034	wwPDB-VP
Average B, all atoms (Å ²)	319.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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	0.43	0/4646	0.69	0/6281
1	B	0.44	0/4153	0.71	1/5616 (0.0%)
1	C	0.44	0/4153	0.74	5/5616 (0.1%)
1	D	0.43	0/4153	0.71	1/5616 (0.0%)
All	All	0.43	0/17105	0.71	7/23129 (0.0%)

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
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	532	LEU	CA-CB-CG	8.33	134.46	115.30
1	C	467	ARG	CB-CG-CD	6.85	129.41	111.60
1	B	271	ILE	CG1-CB-CG2	-6.54	97.01	111.40
1	D	454	LEU	CA-CB-CG	5.93	128.95	115.30
1	C	236	LEU	CA-CB-CG	5.55	128.07	115.30
1	C	465	ALA	C-N-CD	-5.30	108.93	120.60
1	C	240	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	532	LEU	Peptide
1	C	466	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4595	0	4641	128	0
1	B	4105	0	4153	145	0
1	C	4105	0	4153	160	0
1	D	4105	0	4153	141	0
2	A	31	0	12	2	0
2	B	31	0	12	3	0
2	C	31	0	12	1	0
2	D	31	0	12	5	0
All	All	17034	0	17148	538	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 16.

All (538) 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:D:136:THR:O	1:D:164:GLU:N	1.96	0.99
1:B:31:GLU:HA	1:A:272:GLU:HG3	1.44	0.96
1:B:241:VAL:HG22	1:B:252:LEU:HB2	1.46	0.95
1:C:57:GLN:NE2	1:C:65:THR:OG1	2.07	0.87
1:B:26:VAL:HG21	1:B:369:GLU:HB3	1.55	0.87
1:C:59:VAL:HA	1:C:260:GLN:HB3	1.55	0.86
1:A:29:ASN:ND2	1:A:36:THR:OG1	2.09	0.85
1:D:220:ALA:HB2	1:D:327:ALA:HB2	1.58	0.85
1:C:40:ILE:O	1:C:66:LEU:N	2.10	0.85
1:C:326:ASP:HB3	1:C:506:GLY:HA3	1.60	0.84
1:A:241:VAL:HG21	1:A:253:ARG:HG3	1.61	0.83
1:C:281:VAL:HA	1:D:56:ARG:HH12	1.44	0.82
1:C:477:ASP:O	1:C:485:HIS:N	2.12	0.82
1:C:142:VAL:O	1:C:171:GLU:N	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:PRO:HB3	1:D:260:GLN:HG3	1.63	0.81
1:C:241:VAL:HG22	1:C:252:LEU:HB2	1.61	0.81
1:B:237:ILE:HG23	1:B:262:LEU:HD23	1.62	0.80
1:A:34:ARG:NE	1:A:369:GLU:OE2	2.15	0.80
1:B:72:LEU:HD22	1:B:82:VAL:HG22	1.65	0.79
1:C:404:MET:HB2	1:C:619:LEU:HB2	1.63	0.78
1:C:29:ASN:ND2	1:C:36:THR:OG1	2.17	0.77
1:D:244:PHE:CE2	1:D:296:MET:HA	2.19	0.76
1:D:271:ILE:HG23	2:D:701:ATP:N1	2.01	0.76
1:C:479:ASP:OD2	1:C:485:HIS:NE2	2.18	0.76
1:C:94:ILE:HD13	1:C:104:GLU:HB2	1.67	0.76
1:C:194:ASP:HB3	1:C:201:ASP:HB3	1.66	0.76
1:B:146:PHE:HB3	1:B:151:ARG:HG3	1.67	0.76
1:D:242:GLU:O	1:D:246:LYS:N	2.17	0.76
1:A:242:GLU:OE2	1:A:253:ARG:NH2	2.19	0.76
1:C:139:VAL:HG22	1:C:167:ARG:HB2	1.67	0.75
1:C:338:ILE:HG23	1:C:365:VAL:HG21	1.68	0.75
1:B:56:ARG:HB3	1:A:282:ASN:HB3	1.68	0.75
1:C:532:LEU:HA	1:C:535:THR:HB	1.69	0.75
1:C:81:GLU:OE2	1:C:226:HIS:NE2	2.20	0.74
1:A:128:GLU:HG2	1:A:134:PRO:HA	1.69	0.74
1:C:42:TYR:HB2	1:C:64:ASN:HB3	1.69	0.74
1:C:200:PHE:HE1	1:C:319:PRO:HB2	1.51	0.74
1:B:74:GLY:HA3	1:B:150:GLN:HA	1.70	0.74
1:A:40:ILE:O	1:A:66:LEU:N	2.21	0.74
1:C:31:GLU:HA	1:D:345:ARG:NH1	2.03	0.74
1:C:120:LEU:O	1:C:124:LYS:N	2.20	0.73
1:A:13:ASN:HB3	1:A:35:THR:HB	1.69	0.73
1:A:546:THR:O	1:A:550:VAL:N	2.21	0.73
1:D:206:GLU:N	1:D:217:GLU:O	2.18	0.73
1:B:142:VAL:O	1:B:171:GLU:N	2.19	0.73
1:C:31:GLU:HA	1:D:345:ARG:HH12	1.52	0.72
1:B:142:VAL:HG21	1:B:151:ARG:HG2	1.71	0.71
1:B:220:ALA:HA	1:B:506:GLY:HA2	1.71	0.71
1:B:399:LEU:HD13	1:B:484:LEU:HD22	1.72	0.71
1:D:59:VAL:HA	1:D:260:GLN:HB3	1.71	0.71
1:B:56:ARG:HH12	1:A:281:VAL:HA	1.55	0.71
1:C:362:ARG:NH2	1:C:364:ASP:OD2	2.20	0.71
1:D:2:GLY:N	1:D:137:GLU:OE2	2.24	0.70
1:D:283:LEU:HB2	1:D:296:MET:HB3	1.73	0.70
1:B:345:ARG:HH12	1:A:31:GLU:HA	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLY:O	1:A:448:ALA:N	2.21	0.69
1:C:190:ILE:HD13	1:C:207:ILE:HD11	1.75	0.69
1:B:62:PRO:HB3	1:B:260:GLN:HG3	1.75	0.69
1:B:128:GLU:HG2	1:B:134:PRO:HA	1.74	0.69
1:C:188:ARG:NE	1:C:336:ASP:OD2	2.23	0.69
1:C:477:ASP:HB3	1:C:485:HIS:HB2	1.75	0.68
1:D:29:ASN:ND2	1:D:36:THR:OG1	2.19	0.68
1:B:167:ARG:HG3	1:B:382:LEU:HD11	1.75	0.68
1:B:418:ILE:HG21	1:B:482:GLY:HA2	1.75	0.68
1:B:71:ARG:NH1	1:B:198:GLY:O	2.27	0.67
1:B:345:ARG:NH1	1:A:31:GLU:HA	2.08	0.67
1:D:70:LYS:NZ	2:D:701:ATP:O3G	2.25	0.67
1:B:345:ARG:NH2	1:A:31:GLU:O	2.28	0.67
1:C:66:LEU:HB3	1:C:69:ILE:HD11	1.77	0.66
1:A:552:GLU:HA	1:D:532:LEU:HB3	1.78	0.66
1:C:273:LEU:O	1:C:302:ARG:NH2	2.28	0.66
1:C:477:ASP:N	1:C:485:HIS:O	2.28	0.66
1:B:275:SER:OG	1:A:53:PRO:HB3	1.96	0.66
1:B:243:GLU:HB3	1:B:298:ILE:HD13	1.77	0.66
1:B:284:PRO:HG2	1:A:285:TYR:CD1	2.31	0.66
1:D:204:ILE:O	1:D:219:LEU:N	2.27	0.66
1:C:62:PRO:HB2	1:C:90:PRO:HB2	1.78	0.65
1:B:81:GLU:OE2	1:B:225:THR:OG1	2.14	0.65
1:D:467:ARG:HH22	1:D:619:LEU:HD13	1.61	0.65
1:A:528:LYS:HA	1:A:531:GLU:HG2	1.77	0.65
1:B:237:ILE:HG12	1:B:262:LEU:HG	1.78	0.64
1:C:404:MET:SD	1:C:619:LEU:HD12	2.37	0.64
1:C:465:ALA:HB3	1:C:470:PRO:HD3	1.79	0.64
1:C:271:ILE:HG23	2:C:701:ATP:N6	2.11	0.64
1:B:136:THR:O	1:B:164:GLU:N	2.21	0.64
1:B:339:LEU:HD21	1:B:353:VAL:HG21	1.79	0.64
1:A:41:ALA:HB3	1:A:49:LEU:HB2	1.79	0.64
1:B:261:ARG:NH1	1:B:286:ILE:HA	2.13	0.64
1:C:404:MET:N	1:C:619:LEU:O	2.32	0.63
1:D:174:ALA:O	1:D:374:GLY:HA3	1.98	0.63
1:B:200:PHE:HE1	1:B:319:PRO:HB2	1.63	0.63
1:C:162:GLY:HA2	1:B:358:GLY:HA2	1.80	0.63
1:A:220:ALA:HB2	1:A:327:ALA:HB2	1.80	0.63
1:A:341:GLY:O	1:A:367:PRO:HB2	1.98	0.63
1:B:67:PHE:CE2	1:B:263:LYS:HE3	2.33	0.62
1:D:338:ILE:HG23	1:D:365:VAL:HG21	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ALA:HA	1:A:65:THR:HA	1.80	0.62
1:D:220:ALA:HA	1:D:506:GLY:HA2	1.81	0.62
1:D:278:GLN:HA	1:D:301:THR:HA	1.80	0.62
1:D:467:ARG:NH2	1:D:619:LEU:HD13	2.14	0.62
1:C:3:LYS:HA	1:C:383:THR:HG21	1.80	0.62
1:B:144:ALA:HA	1:B:170:ASN:HB2	1.81	0.61
1:D:159:ARG:HG3	1:D:165:VAL:HG23	1.82	0.61
1:B:31:GLU:OE2	1:B:53:PRO:HD3	2.01	0.61
1:A:160:ILE:O	1:D:355:GLU:HG2	2.00	0.61
1:D:337:VAL:HG11	1:D:353:VAL:HG11	1.82	0.61
1:D:479:ASP:OD2	1:D:485:HIS:NE2	2.24	0.61
1:C:166:LYS:O	1:C:167:ARG:NH2	2.30	0.61
1:A:241:VAL:HG22	1:A:252:LEU:HB2	1.83	0.61
1:C:37:PRO:O	1:C:51:GLY:HA2	2.00	0.61
1:B:407:VAL:HG21	1:B:533:VAL:HG11	1.82	0.61
1:A:72:LEU:HD22	1:A:101:ALA:HB1	1.81	0.60
1:B:151:ARG:HH12	1:B:170:ASN:HB3	1.65	0.60
1:C:200:PHE:CE1	1:C:319:PRO:HB2	2.33	0.60
1:A:12:THR:O	1:A:38:SER:N	2.29	0.60
1:A:531:GLU:HA	1:A:534:GLN:HB3	1.83	0.60
1:C:204:ILE:O	1:C:219:LEU:N	2.34	0.60
1:A:232:PHE:CD2	1:A:309:VAL:HG11	2.36	0.60
1:D:142:VAL:O	1:D:171:GLU:N	2.30	0.59
1:B:239:TYR:O	1:B:243:GLU:N	2.21	0.59
1:B:420:THR:HG22	1:B:478:ILE:HB	1.85	0.59
1:C:81:GLU:O	1:C:85:ASP:N	2.33	0.59
1:B:322:VAL:O	1:B:326:ASP:N	2.35	0.59
1:D:243:GLU:O	1:D:247:ASP:N	2.31	0.59
1:B:179:TYR:CD1	1:B:365:VAL:HG22	2.36	0.59
1:D:26:VAL:HG21	1:D:369:GLU:HB3	1.85	0.59
1:A:8:ASP:HA	1:A:141:THR:OG1	2.03	0.59
1:D:74:GLY:HA3	1:D:150:GLN:HA	1.84	0.59
1:D:200:PHE:HE1	1:D:319:PRO:HB2	1.69	0.58
1:B:244:PHE:HB2	1:B:296:MET:HE2	1.85	0.58
1:D:120:LEU:O	1:D:124:LYS:N	2.32	0.58
1:A:77:PHE:HE1	1:A:93:ILE:HG22	1.67	0.58
1:D:167:ARG:HG2	1:D:382:LEU:HD11	1.86	0.58
1:B:86:VAL:HG22	1:B:93:ILE:HB	1.85	0.58
1:B:196:GLY:O	1:B:229:GLY:N	2.28	0.58
1:C:484:LEU:N	1:C:501:ILE:O	2.34	0.57
1:A:41:ALA:O	1:A:49:LEU:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ASN:ND2	1:A:32:GLY:O	2.38	0.57
1:D:354:ALA:HA	1:D:359:LYS:O	2.04	0.57
1:A:256:PRO:O	1:A:260:GLN:N	2.35	0.57
1:A:557:LEU:HD21	1:A:565:ILE:HD12	1.85	0.57
1:C:53:PRO:HB3	1:D:275:SER:OG	2.05	0.57
1:B:155:LYS:HG2	1:B:165:VAL:HG11	1.86	0.57
1:A:2:GLY:N	1:A:137:GLU:OE2	2.38	0.57
1:D:477:ASP:HB3	1:D:485:HIS:HB2	1.85	0.57
1:B:56:ARG:CZ	1:A:282:ASN:H	2.17	0.57
1:D:241:VAL:HG22	1:D:252:LEU:HB2	1.87	0.57
1:C:9:LEU:O	1:C:70:LYS:NZ	2.35	0.57
1:D:471:GLN:HE22	1:D:617:ARG:HH11	1.53	0.57
1:D:244:PHE:HE2	1:D:296:MET:HA	1.66	0.56
1:D:241:VAL:HG13	1:D:251:ASP:HA	1.86	0.56
1:A:114:GLN:HA	1:A:160:ILE:HG21	1.88	0.56
1:A:584:ILE:O	1:A:588:MET:N	2.32	0.56
1:D:59:VAL:HG12	1:D:260:GLN:O	2.06	0.56
1:D:62:PRO:HB3	1:D:260:GLN:CG	2.35	0.56
1:D:242:GLU:OE1	1:D:245:LYS:HD3	2.06	0.56
1:A:421:LYS:HD3	1:A:477:ASP:OD2	2.05	0.56
1:C:240:LEU:HD11	1:C:262:LEU:HD11	1.88	0.55
1:A:174:ALA:O	1:A:374:GLY:HA3	2.05	0.55
1:C:205:ILE:HG12	1:C:218:VAL:HG22	1.88	0.55
1:A:220:ALA:HA	1:A:506:GLY:HA2	1.87	0.55
1:A:37:PRO:O	1:A:51:GLY:HA2	2.06	0.55
1:C:108:GLN:HE22	1:B:310:GLU:CD	2.10	0.55
1:B:143:PRO:HD2	1:B:146:PHE:CD2	2.41	0.55
1:B:174:ALA:O	1:B:374:GLY:HA3	2.06	0.55
1:A:396:PRO:HB2	1:A:512:ILE:HG21	1.88	0.55
1:D:155:LYS:HG2	1:D:165:VAL:HG11	1.89	0.55
1:D:529:PHE:O	1:D:532:LEU:HG	2.06	0.55
1:C:64:ASN:OD1	1:C:105:VAL:HG13	2.06	0.55
1:C:192:VAL:HG21	1:C:205:ILE:HD12	1.87	0.55
1:A:197:GLY:O	1:A:229:GLY:N	2.40	0.55
1:C:41:ALA:HA	1:C:65:THR:HA	1.88	0.55
1:C:82:VAL:O	1:C:86:VAL:N	2.36	0.55
1:A:146:PHE:HB3	1:A:151:ARG:HG3	1.88	0.55
1:A:341:GLY:HA2	2:A:701:ATP:O2A	2.07	0.55
1:A:16:VAL:HG13	1:A:27:LEU:HB2	1.88	0.55
1:A:94:ILE:HD13	1:A:104:GLU:HB2	1.88	0.54
1:B:71:ARG:O	1:B:75:ARG:NE	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASP:OD2	1:A:25:ARG:HD2	2.06	0.54
1:C:31:GLU:OE1	1:C:52:GLN:HG2	2.07	0.54
1:C:240:LEU:HD22	1:C:262:LEU:HD21	1.89	0.54
1:B:143:PRO:HB3	1:B:145:TYR:CE2	2.42	0.54
1:D:402:GLU:HB2	1:D:441:LEU:HD11	1.88	0.54
1:A:240:LEU:HD13	1:A:262:LEU:HD11	1.90	0.54
1:C:431:ASP:OD2	1:C:467:ARG:HG3	2.08	0.54
1:B:271:ILE:HG23	2:B:701:ATP:C6	2.43	0.54
1:C:41:ALA:HB3	1:C:49:LEU:HB2	1.89	0.54
1:B:283:LEU:HB2	1:B:296:MET:HB3	1.90	0.54
1:B:200:PHE:HB3	1:B:227:LEU:HB2	1.90	0.54
1:B:261:ARG:HH12	1:B:286:ILE:HA	1.71	0.54
1:D:206:GLU:HB3	1:D:217:GLU:HB3	1.89	0.54
1:C:16:VAL:HG13	1:C:27:LEU:HB2	1.90	0.53
1:B:244:PHE:CE2	1:B:296:MET:HA	2.43	0.53
1:A:74:GLY:HA3	1:A:150:GLN:HA	1.90	0.53
1:B:175:ALA:HB2	1:B:371:VAL:HG22	1.90	0.53
1:B:317:ILE:HG23	1:B:356:PHE:CE1	2.43	0.53
1:A:543:LEU:HD12	1:A:569:LEU:HD22	1.90	0.53
1:D:202:ILE:HD13	1:D:320:LEU:HD22	1.91	0.53
1:D:244:PHE:CD2	1:D:296:MET:HG3	2.43	0.53
1:B:178:ALA:HB2	1:B:374:GLY:N	2.24	0.53
1:A:339:LEU:HD11	1:A:350:GLN:HG2	1.90	0.53
1:D:477:ASP:O	1:D:485:HIS:N	2.24	0.53
1:D:231:ASP:O	1:D:235:ARG:HG2	2.08	0.53
1:C:196:GLY:O	1:C:229:GLY:N	2.36	0.53
1:B:221:THR:N	1:B:505:SER:O	2.30	0.53
1:B:428:THR:HG21	1:B:462:ILE:HG21	1.91	0.53
1:D:139:VAL:HG22	1:D:167:ARG:HB2	1.90	0.53
1:C:58:ALA:HB2	1:C:65:THR:HG21	1.90	0.53
1:A:102:TRP:CZ2	1:A:111:ALA:HB2	2.44	0.53
1:A:583:ALA:O	1:A:587:LYS:HG2	2.09	0.53
1:C:86:VAL:HA	1:C:93:ILE:HD12	1.89	0.52
1:B:401:ILE:HD11	1:B:426:PHE:CZ	2.44	0.52
1:C:148:ASP:OD2	1:C:485:HIS:CE1	2.62	0.52
1:C:316:SER:O	1:C:320:LEU:HG	2.09	0.52
1:D:125:LYS:HD2	1:D:128:GLU:HB2	1.91	0.52
1:C:7:ILE:HD13	1:C:120:LEU:HD22	1.91	0.52
1:B:241:VAL:HG13	1:B:252:LEU:H	1.74	0.52
1:C:256:PRO:HA	1:C:259:MET:HB2	1.92	0.52
1:C:241:VAL:HG13	1:C:252:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ALA:HB2	1:C:283:LEU:HD11	1.92	0.52
1:C:397:LEU:HD21	1:C:512:ILE:HG23	1.90	0.52
1:B:90:PRO:HB3	1:B:256:PRO:HB3	1.90	0.52
1:D:401:ILE:HA	1:D:439:HIS:O	2.10	0.52
1:B:269:ALA:HB1	1:B:279:THR:HG21	1.92	0.52
1:B:339:LEU:HD13	1:B:344:THR:HB	1.90	0.52
1:B:402:GLU:OE1	1:B:439:HIS:ND1	2.42	0.52
1:A:341:GLY:N	1:A:367:PRO:O	2.39	0.52
1:D:137:GLU:HG2	1:D:166:LYS:HD3	1.90	0.52
1:D:4:ILE:HG12	1:D:137:GLU:HB3	1.91	0.52
1:D:271:ILE:HG23	2:D:701:ATP:C6	2.45	0.52
1:B:244:PHE:HE2	1:B:296:MET:HA	1.74	0.52
1:B:396:PRO:HB2	1:B:512:ILE:HD13	1.92	0.52
1:A:458:ASN:O	1:A:497:GLN:HG3	2.09	0.52
1:C:42:TYR:N	1:C:64:ASN:O	2.39	0.52
1:D:328:GLY:HA3	1:D:508:ASN:ND2	2.25	0.52
1:C:121:LYS:HA	1:C:124:LYS:HB3	1.92	0.51
1:D:90:PRO:HG3	1:D:260:GLN:OE1	2.09	0.51
1:C:4:ILE:O	1:C:379:GLY:HA3	2.10	0.51
1:B:277:GLN:O	1:B:302:ARG:N	2.28	0.51
1:D:395:THR:HG22	1:D:418:ILE:HD11	1.93	0.51
1:C:70:LYS:NZ	1:C:171:GLU:OE2	2.35	0.51
1:C:212:GLY:O	1:C:388:ASP:HB3	2.11	0.51
1:B:26:VAL:HG21	1:B:369:GLU:CB	2.35	0.51
1:C:296:MET:HG3	1:C:298:ILE:HD11	1.92	0.51
1:B:219:LEU:HA	1:B:507:LEU:HB3	1.92	0.51
1:C:138:ALA:O	1:C:166:LYS:N	2.44	0.51
1:C:447:ARG:HD2	1:C:450:ASP:OD2	2.11	0.51
1:C:484:LEU:O	1:C:501:ILE:N	2.32	0.51
1:B:302:ARG:HH12	1:B:347:PRO:HG2	1.75	0.51
1:D:94:ILE:HD13	1:D:104:GLU:HB2	1.92	0.51
1:D:386:VAL:CG1	1:D:389:VAL:HB	2.41	0.51
1:D:204:ILE:HG21	1:D:329:LEU:HD12	1.93	0.50
1:C:256:PRO:O	1:C:260:GLN:HG2	2.11	0.50
1:B:90:PRO:CB	1:B:256:PRO:HB3	2.41	0.50
1:C:139:VAL:HG21	1:C:378:GLN:HG3	1.93	0.50
1:A:400:GLY:O	1:A:441:LEU:N	2.33	0.50
1:D:69:ILE:HG13	1:D:115:ILE:HG21	1.94	0.50
1:C:215:THR:HG22	1:C:390:LEU:HD23	1.93	0.50
1:C:484:LEU:HB3	1:C:501:ILE:HB	1.93	0.50
1:B:469:MET:HB3	1:B:470:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:VAL:HG11	1:C:501:ILE:CD1	2.42	0.50
1:A:338:ILE:HD13	1:A:362:ARG:HB2	1.93	0.50
1:C:174:ALA:O	1:C:374:GLY:HA3	2.11	0.49
1:A:9:LEU:O	1:A:70:LYS:NZ	2.40	0.49
1:A:81:GLU:O	1:A:85:ASP:N	2.45	0.49
1:D:125:LYS:HA	1:D:128:GLU:HB2	1.94	0.49
1:C:34:ARG:NE	1:C:369:GLU:OE2	2.31	0.49
1:C:81:GLU:HA	1:C:84:ARG:HB3	1.94	0.49
1:A:282:ASN:ND2	1:A:297:ASN:OD1	2.45	0.49
1:A:399:LEU:HD13	1:A:484:LEU:HD22	1.94	0.49
1:B:206:GLU:HB2	1:B:219:LEU:HD11	1.93	0.49
1:B:353:VAL:HG13	1:B:357:PHE:CD2	2.48	0.49
1:D:420:THR:HG22	1:D:478:ILE:HD12	1.93	0.49
1:A:316:SER:C	1:A:319:PRO:HD2	2.33	0.49
1:A:407:VAL:HA	1:A:446:LYS:O	2.12	0.49
1:D:243:GLU:HA	1:D:246:LYS:HB2	1.94	0.49
1:C:289:ASP:OD1	1:C:294:LYS:NZ	2.42	0.49
1:B:200:PHE:HE1	1:B:319:PRO:CB	2.26	0.49
1:A:261:ARG:NH1	1:A:284:PRO:O	2.42	0.49
1:C:42:TYR:O	1:C:61:ASN:ND2	2.46	0.49
1:D:243:GLU:HG2	1:D:298:ILE:HG23	1.94	0.49
1:D:477:ASP:N	1:D:485:HIS:O	2.36	0.49
1:A:302:ARG:NH1	1:A:347:PRO:HG2	2.27	0.49
1:D:433:GLN:NE2	1:D:436:VAL:HG12	2.28	0.49
1:C:61:ASN:HD21	1:C:64:ASN:HB2	1.78	0.49
1:C:145:TYR:HD2	1:C:201:ASP:OD1	1.96	0.49
1:C:193:TYR:CE2	1:C:320:LEU:HD21	2.48	0.49
1:B:121:LYS:HG2	1:B:161:ALA:HA	1.94	0.49
1:C:41:ALA:HB1	1:C:57:GLN:NE2	2.28	0.48
1:A:13:ASN:HA	1:A:36:THR:O	2.13	0.48
1:A:138:ALA:O	1:A:166:LYS:N	2.41	0.48
1:B:53:PRO:O	1:B:57:GLN:HG3	2.13	0.48
1:B:344:THR:HA	1:B:349:VAL:HG11	1.95	0.48
1:A:407:VAL:HG22	1:A:529:PHE:CE2	2.48	0.48
1:B:212:GLY:O	1:B:388:ASP:HB3	2.13	0.48
1:A:269:ALA:HB1	1:A:279:THR:HG21	1.95	0.48
1:D:302:ARG:HH12	1:D:347:PRO:HG2	1.79	0.48
1:C:440:VAL:HG11	1:C:501:ILE:HD13	1.95	0.48
1:A:343:GLN:HA	2:A:701:ATP:N3	2.29	0.48
1:C:90:PRO:HG3	1:C:260:GLN:OE1	2.13	0.48
1:B:124:LYS:HD3	1:B:161:ALA:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:THR:HA	1:C:169:ILE:O	2.14	0.48
1:A:141:THR:HB	1:A:171:GLU:HG3	1.96	0.48
1:A:466:PRO:HD2	1:A:469:MET:SD	2.54	0.48
1:D:401:ILE:HG22	1:D:440:VAL:HA	1.96	0.48
1:C:59:VAL:HA	1:C:260:GLN:CB	2.37	0.48
1:A:117:ALA:CB	1:A:160:ILE:HG22	2.44	0.48
1:D:136:THR:HA	1:D:163:LEU:HD23	1.96	0.48
1:D:244:PHE:CE1	1:D:250:ILE:HD12	2.48	0.48
1:C:142:VAL:HG21	1:C:151:ARG:HG2	1.95	0.47
1:C:272:GLU:OE2	1:C:279:THR:HB	2.13	0.47
1:C:399:LEU:CD1	1:C:478:ILE:HD11	2.44	0.47
1:B:4:ILE:HG12	1:B:137:GLU:HB3	1.96	0.47
1:D:221:THR:N	1:D:505:SER:O	2.34	0.47
1:B:195:LEU:HD23	1:B:343:GLN:HB3	1.95	0.47
1:B:216:PHE:O	1:B:392:LEU:HB3	2.14	0.47
1:D:244:PHE:HE1	1:D:250:ILE:HD12	1.79	0.47
1:C:220:ALA:HA	1:C:506:GLY:HA2	1.96	0.47
1:C:298:ILE:N	1:C:298:ILE:HD12	2.30	0.47
1:A:206:GLU:O	1:A:216:PHE:HA	2.13	0.47
1:D:353:VAL:HG11	1:D:361:PRO:HG3	1.94	0.47
1:C:94:ILE:CD1	1:C:104:GLU:HB2	2.43	0.47
1:C:240:LEU:CD1	1:C:262:LEU:HD11	2.44	0.47
1:C:475:THR:O	1:C:486:VAL:HA	2.14	0.47
1:A:256:PRO:HA	1:A:259:MET:HB2	1.96	0.47
1:D:103:VAL:HG22	1:D:110:MET:O	2.15	0.47
1:C:313:VAL:O	1:C:317:ILE:HG12	2.15	0.47
1:B:155:LYS:HE3	1:B:165:VAL:CG1	2.45	0.47
1:D:167:ARG:CG	1:D:382:LEU:HD11	2.44	0.47
1:B:285:TYR:CZ	1:A:292:GLY:HA2	2.50	0.47
1:D:26:VAL:CG2	1:D:369:GLU:HB3	2.44	0.47
1:C:232:PHE:O	1:C:236:LEU:HD22	2.15	0.47
1:B:58:ALA:CB	1:B:65:THR:HG21	2.45	0.47
1:B:277:GLN:HB2	1:A:45:ASP:CG	2.35	0.47
1:A:242:GLU:O	1:A:246:LYS:N	2.46	0.47
1:A:465:ALA:HB1	1:A:469:MET:SD	2.55	0.47
1:D:124:LYS:HD3	1:D:161:ALA:O	2.15	0.47
1:D:427:SER:HB2	1:D:617:ARG:HG2	1.96	0.47
1:B:29:ASN:ND2	1:B:36:THR:OG1	2.45	0.47
1:C:32:GLY:HA3	1:D:366:ASN:ND2	2.30	0.46
1:C:194:ASP:N	1:C:201:ASP:O	2.36	0.46
1:C:318:GLU:O	1:C:322:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:MET:SD	1:B:298:ILE:HD12	2.55	0.46
1:D:15:CYS:SG	1:D:26:VAL:HG13	2.55	0.46
1:D:283:LEU:HD13	1:D:286:ILE:HD13	1.96	0.46
1:C:281:VAL:HA	1:D:56:ARG:NH1	2.21	0.46
1:A:337:VAL:HB	1:A:361:PRO:HA	1.97	0.46
1:D:204:ILE:HG22	1:D:219:LEU:HB2	1.97	0.46
1:C:45:ASP:HB3	1:D:278:GLN:HG2	1.98	0.46
1:C:139:VAL:HG11	1:C:378:GLN:HG2	1.98	0.46
1:B:30:ALA:O	1:A:276:ALA:HB2	2.16	0.46
1:C:237:ILE:HG21	1:C:259:MET:HE1	1.96	0.46
1:B:208:ASP:O	1:B:215:THR:N	2.41	0.46
1:A:397:LEU:HD22	1:A:444:GLU:HG2	1.98	0.46
1:D:476:PHE:CE1	1:D:486:VAL:HG13	2.50	0.46
1:C:396:PRO:HG3	1:C:507:LEU:HG	1.98	0.46
1:A:41:ALA:HB2	1:A:65:THR:HG23	1.98	0.46
1:A:160:ILE:HA	1:D:355:GLU:O	2.14	0.46
1:A:326:ASP:O	1:A:508:ASN:HB2	2.16	0.46
1:A:531:GLU:HA	1:A:534:GLN:CB	2.46	0.46
1:C:63:GLN:HA	1:C:91:PHE:HB3	1.98	0.46
1:A:531:GLU:O	1:A:534:GLN:HB3	2.16	0.46
1:C:255:ASP:O	1:C:259:MET:HG2	2.15	0.46
1:D:59:VAL:HG11	1:D:264:GLU:OE1	2.15	0.46
1:D:141:THR:HA	1:D:169:ILE:O	2.15	0.46
1:C:509:GLU:HA	1:C:512:ILE:HB	1.98	0.45
1:B:54:ALA:O	1:B:58:ALA:N	2.49	0.45
1:D:31:GLU:OE1	1:D:52:GLN:HG2	2.16	0.45
1:D:37:PRO:HG2	1:D:52:GLN:OE1	2.17	0.45
1:A:341:GLY:C	1:A:367:PRO:HB2	2.36	0.45
1:B:244:PHE:HB2	1:B:296:MET:CE	2.44	0.45
1:A:159:ARG:O	1:D:358:GLY:HA2	2.16	0.45
1:C:139:VAL:HG21	1:C:378:GLN:CG	2.46	0.45
1:C:193:TYR:HE2	1:C:320:LEU:HD11	1.81	0.45
1:C:486:VAL:HB	1:C:499:ILE:CG1	2.46	0.45
1:A:75:ARG:HD3	1:A:79:ASP:OD1	2.17	0.45
1:D:119:VAL:O	1:D:123:MET:HG2	2.16	0.45
1:D:401:ILE:HD13	1:D:438:ILE:HG23	1.99	0.45
1:C:31:GLU:O	1:D:345:ARG:NH2	2.46	0.45
1:C:193:TYR:CD2	1:C:320:LEU:HD21	2.51	0.45
1:B:9:LEU:O	1:B:70:LYS:NZ	2.48	0.45
1:B:72:LEU:CD2	1:B:82:VAL:HG22	2.42	0.45
1:C:282:ASN:H	1:D:56:ARG:CZ	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLY:O	1:C:448:ALA:N	2.45	0.45
1:B:262:LEU:HD13	1:B:283:LEU:HD11	1.99	0.45
1:B:428:THR:CG2	1:B:462:ILE:HD13	2.47	0.45
1:C:217:GLU:HB2	1:C:392:LEU:HD23	1.99	0.45
1:A:265:ALA:HB2	1:A:283:LEU:HD21	1.98	0.45
1:D:483:ILE:HG21	1:D:500:THR:HG23	1.98	0.45
1:B:243:GLU:HG2	1:B:298:ILE:CG2	2.47	0.45
1:B:353:VAL:HG13	1:B:357:PHE:CE2	2.51	0.45
1:D:128:GLU:HG2	1:D:133:GLU:O	2.16	0.45
1:B:202:ILE:HG12	1:B:320:LEU:HA	1.99	0.44
1:D:200:PHE:HE1	1:D:319:PRO:CB	2.30	0.44
1:D:237:ILE:HG23	1:D:262:LEU:HD23	1.99	0.44
1:A:546:THR:O	1:A:550:VAL:HG23	2.17	0.44
1:D:67:PHE:CZ	1:D:263:LYS:HE3	2.51	0.44
1:D:235:ARG:NH1	1:D:308:LEU:O	2.46	0.44
1:B:4:ILE:HA	1:B:137:GLU:O	2.18	0.44
1:C:213:GLU:OE1	1:C:390:LEU:HB2	2.17	0.44
1:B:57:GLN:HB3	1:A:282:ASN:ND2	2.31	0.44
1:B:532:LEU:HA	1:B:535:THR:HB	2.00	0.44
1:A:81:GLU:O	1:A:85:ASP:HB2	2.18	0.44
1:A:200:PHE:CE1	1:A:319:PRO:HB2	2.52	0.44
1:A:542:LEU:HG	1:A:591:LEU:HD23	1.99	0.44
1:C:397:LEU:HD11	1:C:512:ILE:HG12	2.00	0.44
1:B:243:GLU:HG2	1:B:298:ILE:HG23	1.98	0.44
1:A:5:ILE:HG12	1:A:137:GLU:O	2.18	0.44
1:A:81:GLU:HA	1:A:84:ARG:HB3	1.98	0.44
1:A:200:PHE:HE1	1:A:319:PRO:HB2	1.83	0.44
1:A:160:ILE:HG23	1:D:355:GLU:HB3	1.99	0.44
1:D:222:ASN:ND2	1:D:319:PRO:O	2.46	0.44
1:D:302:ARG:NH1	1:D:347:PRO:HG2	2.33	0.44
1:C:42:TYR:CD2	1:C:105:VAL:HG11	2.53	0.44
1:C:192:VAL:HB	1:C:203:SER:HB2	2.00	0.44
1:C:476:PHE:CD2	1:C:484:LEU:HD11	2.53	0.44
1:C:235:ARG:O	1:C:236:LEU:HD13	2.18	0.44
1:B:17:ALA:HB2	1:B:26:VAL:HG22	2.00	0.44
1:C:81:GLU:O	1:C:84:ARG:HB3	2.18	0.43
1:A:317:ILE:HG23	1:A:356:PHE:CE1	2.53	0.43
1:D:31:GLU:OE2	1:D:52:GLN:HB3	2.17	0.43
1:D:136:THR:HA	1:D:163:LEU:HA	2.00	0.43
1:C:427:SER:OG	1:C:468:GLY:HA2	2.18	0.43
1:D:40:ILE:HD13	1:D:115:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:PHE:CE1	1:D:319:PRO:HB2	2.51	0.43
1:D:271:ILE:HG12	2:D:701:ATP:C2	2.51	0.43
1:C:68:ALA:HB2	1:C:230:GLU:OE2	2.18	0.43
1:C:478:ILE:HA	1:C:483:ILE:O	2.18	0.43
1:C:483:ILE:HG12	1:C:503:ALA:H	1.83	0.43
1:B:4:ILE:HG21	1:B:139:VAL:HG23	1.99	0.43
1:B:11:THR:OG1	1:B:70:LYS:HB3	2.19	0.43
1:B:278:GLN:HA	1:B:301:THR:HA	2.01	0.43
1:D:5:ILE:HD13	1:D:135:VAL:HG11	2.00	0.43
1:D:256:PRO:HA	1:D:259:MET:HB2	2.01	0.43
1:C:24:PRO:HD3	1:C:181:LEU:HD13	1.98	0.43
1:D:196:GLY:HA3	2:D:701:ATP:O3B	2.19	0.43
1:D:398:SER:HA	1:D:412:ILE:O	2.19	0.43
1:C:3:LYS:HA	1:C:383:THR:CG2	2.45	0.43
1:B:305:LEU:O	1:B:309:VAL:HG22	2.18	0.43
1:D:475:THR:HB	1:D:487:SER:OG	2.17	0.43
1:C:96:ALA:HB2	1:C:102:TRP:CD1	2.53	0.43
1:C:179:TYR:HE1	1:C:362:ARG:CZ	2.31	0.43
1:B:155:LYS:HE3	1:B:165:VAL:HG11	2.01	0.43
1:B:288:ALA:HA	1:B:293:PRO:HA	2.01	0.43
1:D:513:GLN:O	1:D:517:ARG:HG3	2.18	0.43
1:C:49:LEU:C	1:C:54:ALA:HB2	2.38	0.43
1:C:27:LEU:HD22	1:C:130:TYR:CZ	2.54	0.43
1:C:194:ASP:O	1:C:201:ASP:N	2.47	0.43
1:C:200:PHE:HE1	1:C:319:PRO:CB	2.27	0.43
1:C:379:GLY:O	1:C:383:THR:HG23	2.19	0.43
1:B:255:ASP:O	1:B:259:MET:HG2	2.19	0.43
1:C:418:ILE:HG21	1:C:482:GLY:HA2	2.00	0.42
1:B:119:VAL:O	1:B:123:MET:HG2	2.18	0.42
1:C:216:PHE:O	1:C:392:LEU:HB3	2.18	0.42
1:A:241:VAL:HG13	1:A:252:LEU:H	1.83	0.42
1:D:241:VAL:O	1:D:245:LYS:HB2	2.19	0.42
1:A:11:THR:O	1:A:38:SER:HB2	2.18	0.42
1:D:244:PHE:HB2	1:D:298:ILE:HD11	2.01	0.42
1:D:475:THR:O	1:D:486:VAL:HA	2.19	0.42
1:A:124:LYS:HG3	1:A:135:VAL:O	2.19	0.42
1:D:337:VAL:HG11	1:D:353:VAL:CG1	2.49	0.42
1:D:380:GLY:O	1:D:384:GLY:N	2.51	0.42
1:D:486:VAL:HB	1:D:499:ILE:CG1	2.49	0.42
1:C:395:THR:HG22	1:C:418:ILE:HD11	2.02	0.42
1:C:35:THR:HG21	1:C:368:ASP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:HA	1:B:93:ILE:HD12	2.01	0.42
1:B:418:ILE:HG12	1:B:478:ILE:HG21	2.01	0.42
1:C:293:PRO:HD3	1:D:285:TYR:CE1	2.55	0.42
1:B:73:ILE:O	1:B:150:GLN:HG2	2.19	0.42
1:B:398:SER:HA	1:B:412:ILE:O	2.19	0.42
1:D:421:LYS:HD3	1:D:477:ASP:OD2	2.20	0.42
1:B:19:MET:HG2	1:B:376:ALA:O	2.19	0.42
1:B:56:ARG:NH1	1:A:282:ASN:H	2.17	0.42
1:B:196:GLY:HA3	2:B:701:ATP:O3B	2.19	0.42
1:B:167:ARG:CG	1:B:382:LEU:HD11	2.47	0.42
1:B:363:LYS:HD2	1:A:129:ASP:OD2	2.19	0.42
1:B:465:ALA:HB3	1:B:470:PRO:HG3	2.02	0.42
1:D:6:GLY:HA3	1:D:376:ALA:N	2.34	0.42
1:C:142:VAL:O	1:C:170:ASN:HA	2.19	0.42
1:B:58:ALA:HB1	1:B:65:THR:HG21	2.02	0.42
1:A:50:VAL:HG13	1:A:119:VAL:HG22	2.01	0.42
1:A:96:ALA:HB2	1:A:102:TRP:CD2	2.54	0.42
1:D:17:ALA:HB3	1:D:372:ALA:C	2.39	0.42
1:C:61:ASN:ND2	1:C:64:ASN:HB2	2.35	0.41
1:A:160:ILE:HA	1:D:355:GLU:HA	2.01	0.41
1:A:12:THR:O	1:A:37:PRO:HA	2.20	0.41
1:A:373:ILE:O	1:A:377:VAL:HG23	2.20	0.41
1:D:306:GLU:O	1:D:310:GLU:HB2	2.19	0.41
1:C:96:ALA:HB2	1:C:102:TRP:CE2	2.55	0.41
1:A:179:TYR:OH	1:A:362:ARG:NH1	2.52	0.41
1:C:96:ALA:HB2	1:C:102:TRP:CD2	2.55	0.41
1:C:162:GLY:HA2	1:B:358:GLY:CA	2.49	0.41
1:C:399:LEU:HD13	1:C:484:LEU:HD22	2.02	0.41
1:B:412:ILE:HD11	1:B:476:PHE:HB3	2.02	0.41
1:B:12:THR:HB	2:B:701:ATP:H3'	2.02	0.41
1:B:531:GLU:O	1:B:534:GLN:HB3	2.19	0.41
1:A:4:ILE:HB	1:A:379:GLY:CA	2.51	0.41
1:A:272:GLU:OE2	1:A:279:THR:OG1	2.36	0.41
1:D:96:ALA:HB2	1:D:102:TRP:CE2	2.55	0.41
1:C:262:LEU:HD12	1:C:262:LEU:HA	1.85	0.41
1:B:15:CYS:HB2	1:B:35:THR:HG22	2.02	0.41
1:B:75:ARG:HH22	1:B:225:THR:HG21	1.86	0.41
1:B:82:VAL:O	1:B:86:VAL:HG23	2.20	0.41
1:A:49:LEU:HD12	1:A:57:GLN:HG2	2.03	0.41
1:D:50:VAL:HG12	1:D:122:LYS:HD3	2.01	0.41
1:C:302:ARG:HH12	1:C:347:PRO:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ALA:HB2	1:B:370:ALA:O	2.20	0.41
1:B:285:TYR:CG	1:A:293:PRO:HD3	2.55	0.41
1:A:117:ALA:HA	1:A:161:ALA:HB2	2.02	0.41
1:A:302:ARG:HH12	1:A:347:PRO:HG2	1.84	0.41
1:D:241:VAL:O	1:D:245:LYS:N	2.43	0.41
1:C:189:THR:HG21	1:C:329:LEU:CD1	2.50	0.41
1:A:34:ARG:NH2	1:A:369:GLU:OE1	2.54	0.41
1:B:81:GLU:OE2	1:B:226:HIS:NE2	2.54	0.41
1:A:525:ALA:O	1:A:528:LYS:HG3	2.21	0.41
1:D:3:LYS:O	1:D:137:GLU:HB2	2.21	0.41
1:C:40:ILE:HB	1:C:66:LEU:HB2	2.02	0.41
1:B:440:VAL:HG12	1:B:454:LEU:HD12	2.03	0.41
1:A:469:MET:HB3	1:A:470:PRO:HD3	2.02	0.41
1:D:81:GLU:O	1:D:85:ASP:HB2	2.21	0.41
1:B:283:LEU:HD13	1:B:286:ILE:HD13	2.03	0.40
1:A:113:PRO:HB2	1:A:160:ILE:HD12	2.03	0.40
1:A:462:ILE:HG12	1:A:490:ASP:OD2	2.21	0.40
1:D:13:ASN:HB3	1:D:35:THR:HB	2.04	0.40
1:B:396:PRO:CB	1:B:512:ILE:HD13	2.50	0.40
1:B:426:PHE:HB3	1:B:620:LEU:HG	2.03	0.40
1:A:251:ASP:O	1:A:254:ASN:ND2	2.54	0.40
1:A:281:VAL:O	1:A:297:ASN:HA	2.21	0.40
1:D:529:PHE:HA	1:D:532:LEU:CD2	2.50	0.40
1:C:192:VAL:CG2	1:C:205:ILE:HD12	2.50	0.40
1:C:214:LYS:HG2	1:C:216:PHE:CE1	2.56	0.40
1:B:52:GLN:O	1:B:56:ARG:HG3	2.21	0.40
1:B:62:PRO:HG3	1:B:257:LEU:HD23	2.02	0.40
1:D:206:GLU:HB2	1:D:219:LEU:HD21	2.03	0.40
1:C:234:SER:C	1:C:236:LEU:H	2.25	0.40
1:B:294:LYS:HA	1:B:294:LYS:HD3	1.88	0.40
1:B:428:THR:HG22	1:B:462:ILE:HD13	2.03	0.40
1:D:26:VAL:HG21	1:D:369:GLU:OE1	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	604/622 (97%)	597 (99%)	6 (1%)	1 (0%)	47	81
1	B	537/622 (86%)	532 (99%)	5 (1%)	0	100	100
1	C	537/622 (86%)	528 (98%)	8 (2%)	1 (0%)	47	81
1	D	537/622 (86%)	532 (99%)	5 (1%)	0	100	100
All	All	2215/2488 (89%)	2189 (99%)	24 (1%)	2 (0%)	51	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	VAL
1	C	235	ARG

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	492/506 (97%)	486 (99%)	6 (1%)	71	83
1	B	443/506 (88%)	441 (100%)	2 (0%)	88	93
1	C	443/506 (88%)	434 (98%)	9 (2%)	55	74
1	D	443/506 (88%)	438 (99%)	5 (1%)	73	84
All	All	1821/2024 (90%)	1799 (99%)	22 (1%)	71	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	236	LEU
1	C	273	LEU
1	C	298	ILE
1	C	305	LEU

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Mol	Chain	Res	Type
1	C	346	MET
1	C	466	PRO
1	C	467	ARG
1	C	528	LYS
1	C	534	GLN
1	B	528	LYS
1	B	534	GLN
1	A	146	PHE
1	A	297	ASN
1	A	528	LYS
1	A	534	GLN
1	A	598	LEU
1	A	600	GLU
1	D	19	MET
1	D	25	ARG
1	D	385	ASP
1	D	528	LYS
1	D	534	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	108	GLN
1	B	451	ASN
1	A	29	ASN
1	A	282	ASN
1	D	451	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	C	701	-	26,33,33	1.36	4 (15%)	31,52,52	1.71	6 (19%)
2	ATP	A	701	-	26,33,33	1.05	1 (3%)	31,52,52	1.29	3 (9%)
2	ATP	B	701	-	26,33,33	1.17	3 (11%)	31,52,52	1.47	4 (12%)
2	ATP	D	701	-	26,33,33	1.14	3 (11%)	31,52,52	1.57	5 (16%)

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	C	701	-	-	0/18/38/38	0/3/3/3
2	ATP	A	701	-	-	0/18/38/38	0/3/3/3
2	ATP	B	701	-	-	0/18/38/38	0/3/3/3
2	ATP	D	701	-	-	0/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	ATP	C5-C4	3.74	1.50	1.40
2	B	701	ATP	C5-C4	3.01	1.48	1.40
2	A	701	ATP	C5-C4	2.93	1.48	1.40
2	D	701	ATP	C5-C4	2.83	1.48	1.40
2	C	701	ATP	C2-N3	2.55	1.36	1.32
2	B	701	ATP	O4'-C1'	2.44	1.44	1.41
2	C	701	ATP	C6-C5	2.30	1.51	1.43
2	B	701	ATP	C2-N3	2.24	1.35	1.32
2	C	701	ATP	C2-N1	2.12	1.37	1.33
2	D	701	ATP	O4'-C1'	2.06	1.44	1.41
2	D	701	ATP	C6-C5	2.05	1.50	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	ATP	N3-C2-N1	-4.93	120.98	128.68
2	C	701	ATP	C2-N1-C6	4.20	125.94	118.75
2	B	701	ATP	C4-C5-N7	-3.87	105.37	109.40
2	D	701	ATP	C4-C5-N7	-3.69	105.55	109.40
2	A	701	ATP	N3-C2-N1	-3.51	123.20	128.68
2	A	701	ATP	C4-C5-N7	-3.35	105.91	109.40
2	D	701	ATP	N3-C2-N1	-3.34	123.46	128.68
2	B	701	ATP	O2A-PA-O5'	3.23	122.73	107.75
2	B	701	ATP	N3-C2-N1	-2.99	124.00	128.68
2	B	701	ATP	O4'-C1'-C2'	-2.94	102.62	106.93
2	C	701	ATP	C4-C5-N7	-2.88	106.40	109.40
2	D	701	ATP	O2A-PA-O5'	2.70	120.30	107.75
2	D	701	ATP	C5-C6-N6	2.68	124.42	120.35
2	D	701	ATP	C2-N1-C6	2.64	123.28	118.75
2	C	701	ATP	C5-C6-N1	-2.54	114.59	120.35
2	A	701	ATP	C2-N1-C6	2.52	123.07	118.75
2	C	701	ATP	O3'-C3'-C2'	-2.27	104.47	111.82
2	C	701	ATP	C5-C6-N6	2.11	123.55	120.35

There are no chirality outliers.

There are no torsion outliers.

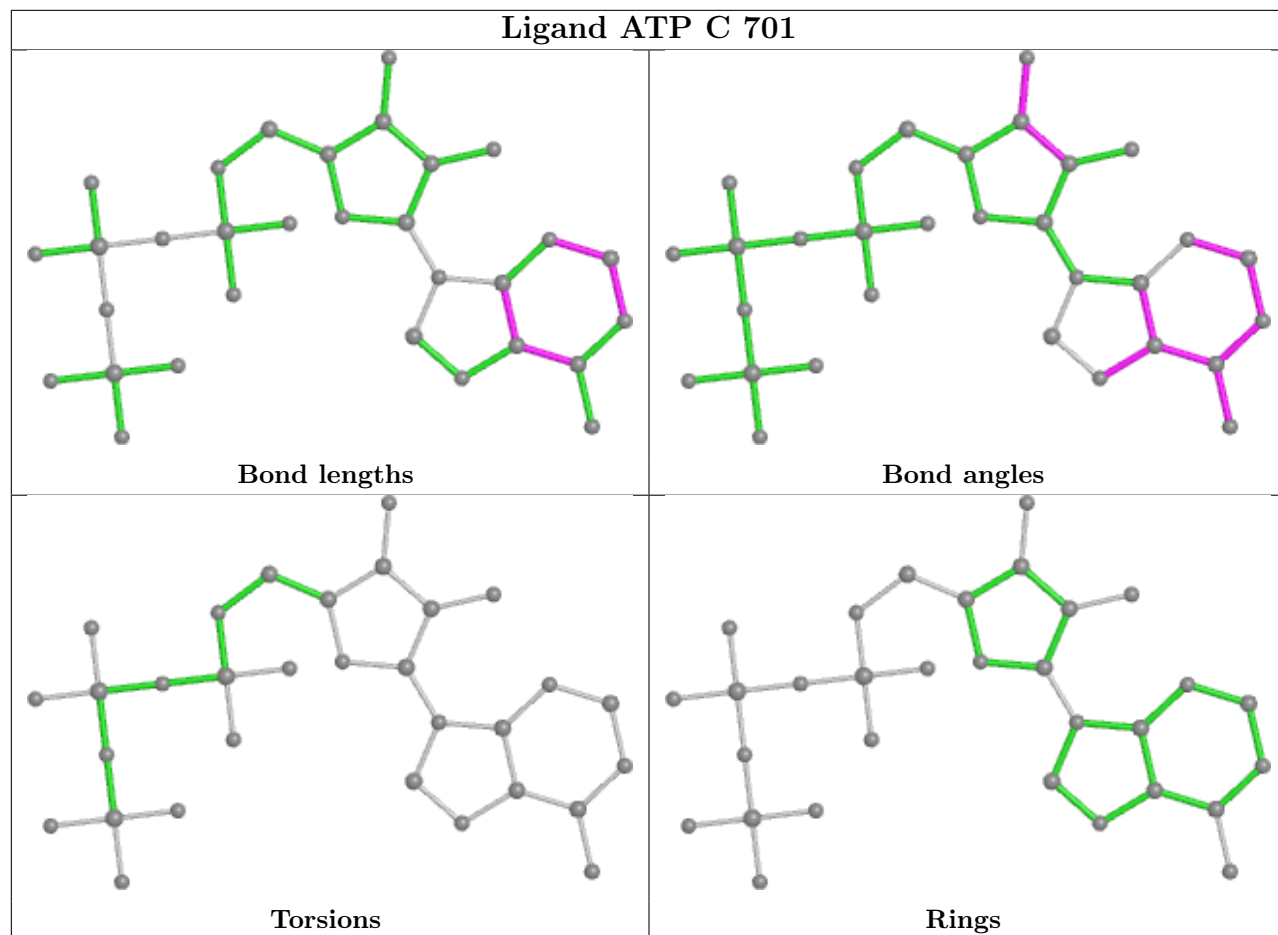
There are no ring outliers.

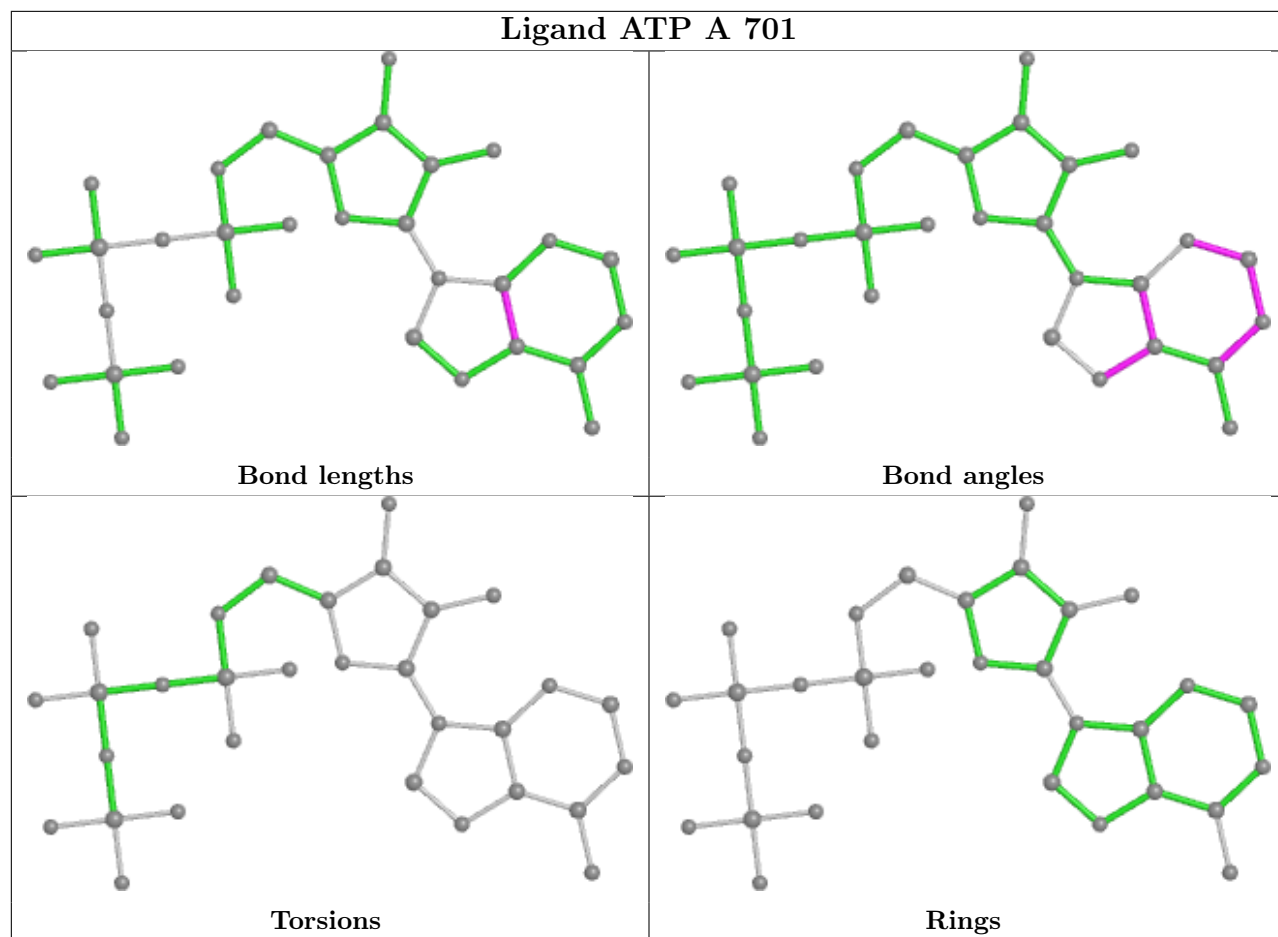
4 monomers are involved in 11 short contacts:

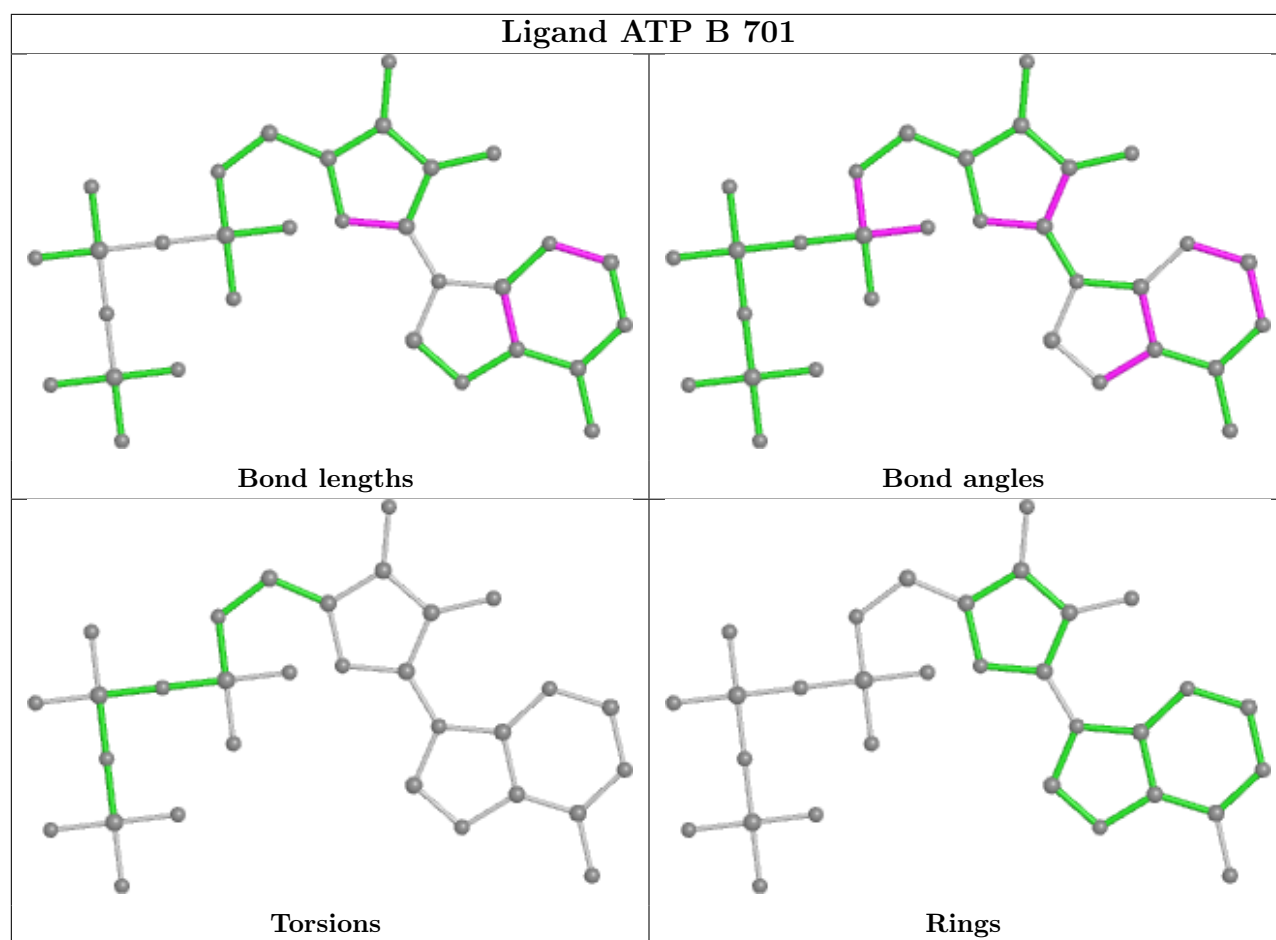
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	ATP	1	0
2	A	701	ATP	2	0
2	B	701	ATP	3	0
2	D	701	ATP	5	0

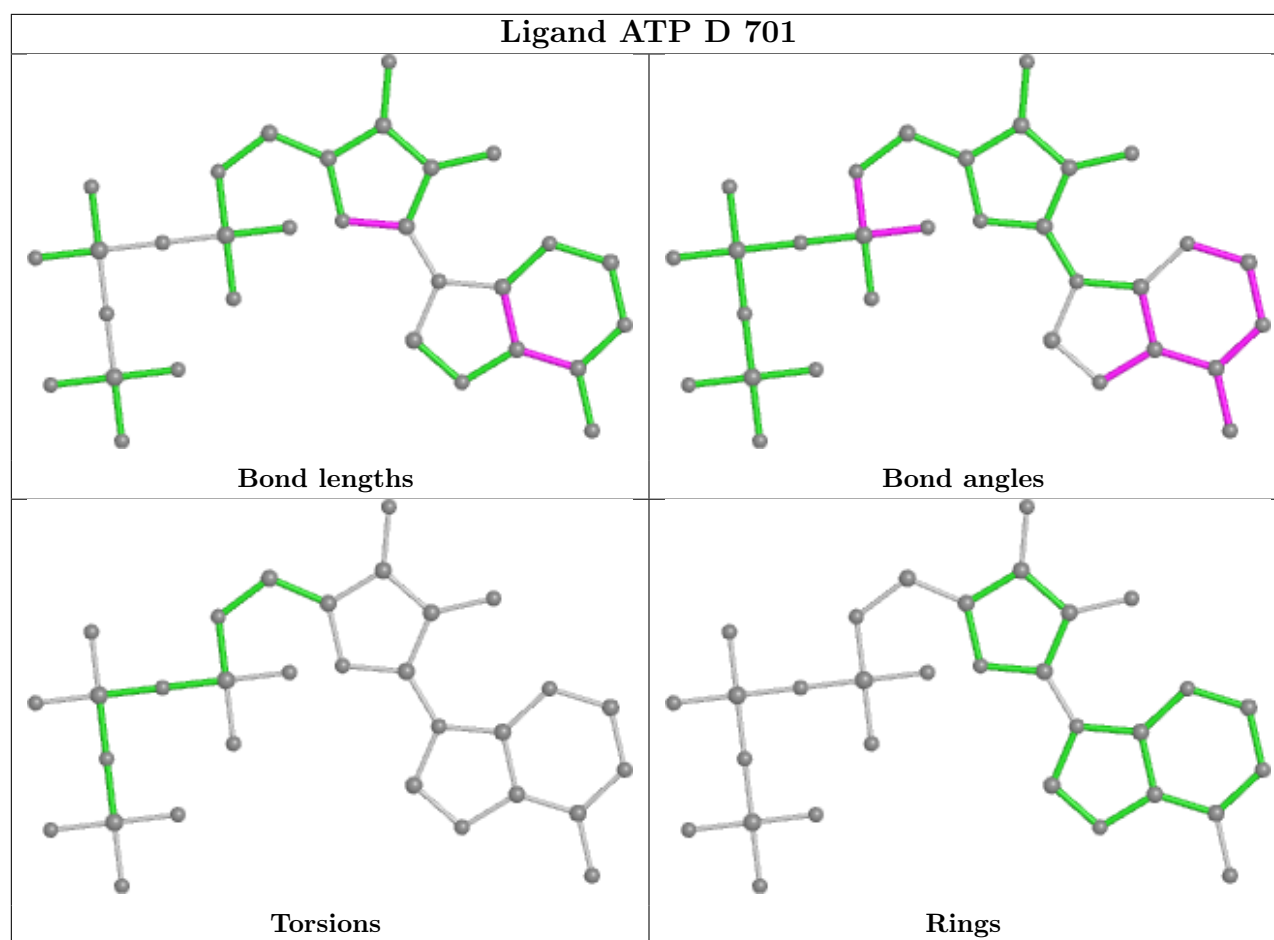
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	608/622 (97%)	2.23	269 (44%) 0 1	320, 320, 320, 320	0
1	B	541/622 (86%)	2.18	240 (44%) 0 1	320, 320, 320, 320	0
1	C	541/622 (86%)	2.08	232 (42%) 0 1	320, 320, 320, 320	0
1	D	541/622 (86%)	2.11	236 (43%) 0 1	320, 320, 320, 320	0
All	All	2231/2488 (89%)	2.15	977 (43%) 0 1	320, 320, 320, 320	0

All (977) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	619	LEU	16.6
1	A	620	LEU	14.8
1	A	552	GLU	13.3
1	B	488	ALA	12.5
1	A	621	THR	12.3
1	D	24	PRO	12.2
1	C	400	GLY	11.7
1	A	28	GLU	11.3
1	D	463	ASN	10.9
1	B	487	SER	10.9
1	A	403	THR	10.7
1	A	191	ALA	10.3
1	D	191	ALA	10.0
1	C	443	GLY	9.9
1	A	29	ASN	9.9
1	A	338	ILE	9.9
1	B	403	THR	9.7
1	B	409	THR	9.4
1	B	205	ILE	9.2
1	A	429	ALA	9.1
1	A	428	THR	9.0

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Mol	Chain	Res	Type	RSRZ
1	D	25	ARG	8.9
1	C	68	ALA	8.8
1	D	66	LEU	8.8
1	B	424	GLN	8.8
1	B	497	GLN	8.7
1	D	500	THR	8.7
1	C	442	GLN	8.6
1	C	411	LEU	8.5
1	C	340	VAL	8.5
1	C	396	PRO	8.5
1	B	191	ALA	8.5
1	D	23	THR	8.5
1	D	194	ASP	8.4
1	A	27	LEU	8.3
1	A	404	MET	8.3
1	B	474	VAL	8.2
1	A	551	GLU	8.1
1	A	549	GLN	8.1
1	A	618	LEU	8.0
1	C	444	GLU	8.0
1	D	67	PHE	8.0
1	D	495	LYS	8.0
1	D	403	THR	8.0
1	A	598	LEU	7.8
1	D	20	ASP	7.8
1	C	338	ILE	7.8
1	A	402	GLU	7.7
1	D	499	ILE	7.6
1	C	398	SER	7.6
1	A	553	ALA	7.6
1	D	493	SER	7.6
1	B	40	ILE	7.5
1	A	391	LEU	7.5
1	C	339	LEU	7.5
1	C	399	LEU	7.4
1	A	33	ASP	7.4
1	B	5	ILE	7.4
1	A	192	VAL	7.4
1	C	423	SER	7.3
1	D	192	VAL	7.3
1	A	513	GLN	7.3
1	B	444	GLU	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	395	THR	7.2
1	B	431	ASP	7.2
1	A	595	SER	7.1
1	A	34	ARG	7.1
1	C	74	GLY	7.1
1	B	203	SER	7.0
1	D	462	ILE	7.0
1	D	464	PRO	6.9
1	B	217	GLU	6.9
1	A	409	THR	6.9
1	B	404	MET	6.9
1	C	409	THR	6.9
1	C	410	THR	6.8
1	A	389	VAL	6.8
1	D	494	GLY	6.8
1	B	407	VAL	6.8
1	A	193	TYR	6.8
1	B	232	PHE	6.7
1	B	192	VAL	6.7
1	C	73	ILE	6.7
1	D	193	TYR	6.7
1	D	337	VAL	6.7
1	A	622	GLY	6.7
1	C	397	LEU	6.7
1	C	37	PRO	6.7
1	C	191	ALA	6.6
1	A	427	SER	6.6
1	B	486	VAL	6.6
1	A	433	GLN	6.6
1	B	393	ASP	6.5
1	A	550	VAL	6.5
1	C	424	GLN	6.5
1	D	501	ILE	6.5
1	D	68	ALA	6.5
1	C	72	LEU	6.4
1	B	443	GLY	6.4
1	A	337	VAL	6.4
1	C	75	ARG	6.4
1	C	359	LYS	6.3
1	C	337	VAL	6.3
1	A	393	ASP	6.3
1	D	460	ASP	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	426	PHE	6.3
1	B	218	VAL	6.2
1	A	512	ILE	6.2
1	B	206	GLU	6.2
1	A	435	ALA	6.2
1	B	190	ILE	6.2
1	B	233	ASP	6.2
1	C	360	GLU	6.2
1	B	406	GLY	6.1
1	D	21	GLY	6.1
1	D	391	LEU	6.1
1	D	405	GLY	6.1
1	C	358	GLY	6.0
1	B	446	LYS	6.0
1	D	461	GLY	6.0
1	C	176	ALA	6.0
1	B	4	ILE	6.0
1	D	423	SER	6.0
1	D	40	ILE	6.0
1	A	30	ALA	5.9
1	A	216	PHE	5.9
1	D	404	MET	5.9
1	A	35	THR	5.9
1	D	338	ILE	5.9
1	B	204	ILE	5.9
1	D	172	PRO	5.8
1	D	22	THR	5.8
1	B	426	PHE	5.8
1	C	526	ASP	5.8
1	A	453	SER	5.8
1	B	425	VAL	5.8
1	B	112	PRO	5.8
1	A	201	ASP	5.8
1	C	365	VAL	5.7
1	D	393	ASP	5.7
1	A	214	LYS	5.7
1	C	112	PRO	5.7
1	A	405	GLY	5.7
1	B	618	LEU	5.7
1	C	394	VAL	5.7
1	A	392	LEU	5.7
1	A	31	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	267	GLU	5.6
1	B	455	GLY	5.6
1	B	156	ASP	5.6
1	B	113	PRO	5.6
1	B	50	VAL	5.5
1	C	357	PHE	5.5
1	D	18	ILE	5.5
1	D	336	ASP	5.5
1	A	26	VAL	5.5
1	C	69	ILE	5.5
1	A	548	LYS	5.5
1	A	130	TYR	5.5
1	B	391	LEU	5.5
1	A	396	PRO	5.5
1	B	496	GLU	5.4
1	C	416	THR	5.4
1	A	357	PHE	5.4
1	B	173	THR	5.4
1	A	331	VAL	5.4
1	B	392	LEU	5.4
1	B	401	ILE	5.4
1	B	66	LEU	5.4
1	A	467	ARG	5.3
1	A	547	ARG	5.3
1	B	617	ARG	5.3
1	D	424	GLN	5.3
1	B	410	THR	5.3
1	C	361	PRO	5.3
1	C	175	ALA	5.3
1	A	436	VAL	5.3
1	C	67	PHE	5.3
1	A	530	GLU	5.3
1	B	118	GLU	5.3
1	B	157	ALA	5.3
1	D	269	ALA	5.3
1	D	528	LYS	5.3
1	B	160	ILE	5.2
1	A	217	GLU	5.2
1	C	353	VAL	5.2
1	B	402	GLU	5.2
1	C	422	HIS	5.2
1	D	485	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	194	ASP	5.2
1	B	494	GLY	5.2
1	B	154	THR	5.2
1	B	473	GLU	5.2
1	C	52	GLN	5.2
1	B	619	LEU	5.1
1	A	190	ILE	5.1
1	D	89	MET	5.1
1	B	116	SER	5.0
1	D	270	LYS	5.0
1	C	24	PRO	5.0
1	B	379	GLY	5.0
1	C	5	ILE	5.0
1	B	219	LEU	5.0
1	B	396	PRO	5.0
1	A	336	ASP	5.0
1	D	201	ASP	5.0
1	A	215	THR	5.0
1	A	199	ALA	5.0
1	B	523	ALA	5.0
1	C	217	GLU	5.0
1	B	467	ARG	5.0
1	D	168	ILE	5.0
1	B	73	ILE	4.9
1	B	503	ALA	4.9
1	D	195	LEU	4.9
1	A	395	THR	4.9
1	C	427	SER	4.9
1	B	405	GLY	4.9
1	A	430	GLU	4.9
1	B	216	PHE	4.8
1	A	390	LEU	4.8
1	B	489	LYS	4.8
1	B	502	LYS	4.8
1	A	401	ILE	4.8
1	A	516	VAL	4.8
1	A	71	ARG	4.8
1	B	115	ILE	4.8
1	C	401	ILE	4.8
1	D	490	ASP	4.8
1	B	220	ALA	4.8
1	B	193	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	423	SER	4.7
1	C	415	ASN	4.7
1	D	484	LEU	4.7
1	C	350	GLN	4.7
1	A	410	THR	4.7
1	B	39	ILE	4.7
1	C	230	GLU	4.7
1	D	266	ALA	4.7
1	B	338	ILE	4.7
1	C	267	GLU	4.7
1	D	133	GLU	4.7
1	A	546	THR	4.7
1	C	522	ASN	4.7
1	C	263	LYS	4.6
1	D	190	ILE	4.6
1	B	495	LYS	4.6
1	A	68	ALA	4.6
1	C	440	VAL	4.6
1	C	441	LEU	4.6
1	B	408	MET	4.6
1	B	445	ARG	4.6
1	C	111	ALA	4.6
1	C	445	ARG	4.6
1	C	412	ILE	4.6
1	A	32	GLY	4.6
1	A	597	LYS	4.6
1	C	56	ARG	4.6
1	C	364	ASP	4.6
1	B	475	THR	4.6
1	D	496	GLU	4.6
1	C	250	ILE	4.6
1	D	432	ASN	4.6
1	C	504	SER	4.5
1	D	497	GLN	4.5
1	A	69	ILE	4.5
1	C	173	THR	4.5
1	D	39	ILE	4.5
1	A	503	ALA	4.5
1	B	207	ILE	4.5
1	D	533	VAL	4.5
1	C	474	VAL	4.5
1	B	499	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	490	ASP	4.5
1	A	266	ALA	4.5
1	C	193	TYR	4.5
1	D	486	VAL	4.5
1	C	414	LYS	4.4
1	D	442	GLN	4.4
1	A	394	VAL	4.4
1	D	171	GLU	4.4
1	C	472	ILE	4.4
1	A	432	ASN	4.4
1	D	170	ASN	4.4
1	C	264	GLU	4.4
1	B	172	PRO	4.4
1	D	26	VAL	4.4
1	C	356	PHE	4.4
1	D	465	ALA	4.4
1	A	596	GLN	4.4
1	D	498	LYS	4.3
1	A	226	HIS	4.3
1	A	198	GLY	4.3
1	C	425	VAL	4.3
1	A	463	ASN	4.3
1	B	398	SER	4.3
1	D	272	GLU	4.3
1	D	532	LEU	4.3
1	A	388	ASP	4.3
1	A	451	ASN	4.3
1	B	155	LYS	4.3
1	A	426	PHE	4.3
1	C	298	ILE	4.3
1	B	427	SER	4.3
1	B	493	SER	4.3
1	B	429	ALA	4.3
1	C	115	ILE	4.2
1	B	456	GLN	4.2
1	A	480	ALA	4.2
1	A	556	LYS	4.2
1	D	93	ILE	4.2
1	B	117	ALA	4.2
1	A	176	ALA	4.2
1	C	262	LEU	4.2
1	B	270	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	264	GLU	4.2
1	C	51	GLY	4.2
1	C	417	THR	4.2
1	B	378	GLN	4.2
1	A	129	ASP	4.2
1	A	223	GLY	4.2
1	C	413	ALA	4.2
1	D	459	LEU	4.2
1	C	177	LEU	4.2
1	B	313	VAL	4.2
1	C	349	VAL	4.2
1	C	525	ALA	4.2
1	A	203	SER	4.2
1	B	67	PHE	4.1
1	A	599	MET	4.1
1	D	529	PHE	4.1
1	C	527	ARG	4.1
1	A	265	ALA	4.1
1	C	391	LEU	4.1
1	B	522	ASN	4.1
1	A	537	ASN	4.1
1	A	531	GLU	4.1
1	C	232	PHE	4.1
1	C	473	GLU	4.1
1	A	225	THR	4.1
1	D	431	ASP	4.1
1	A	617	ARG	4.1
1	D	406	GLY	4.1
1	B	140	ILE	4.1
1	B	428	THR	4.1
1	A	439	HIS	4.1
1	A	515	MET	4.1
1	A	63	GLN	4.0
1	B	504	SER	4.0
1	D	526	ASP	4.0
1	C	355	GLU	4.0
1	C	192	VAL	4.0
1	B	457	PHE	4.0
1	D	140	ILE	4.0
1	A	545	SER	4.0
1	A	533	VAL	4.0
1	A	213	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	336	ASP	4.0
1	B	267	GLU	4.0
1	C	352	LYS	3.9
1	C	38	SER	3.9
1	A	308	LEU	3.9
1	A	462	ILE	3.9
1	D	85	ASP	3.9
1	A	173	THR	3.9
1	D	331	VAL	3.9
1	B	159	ARG	3.9
1	B	264	GLU	3.9
1	C	235	ARG	3.9
1	C	265	ALA	3.9
1	D	141	THR	3.9
1	D	91	PHE	3.9
1	A	397	LEU	3.9
1	A	24	PRO	3.9
1	D	203	SER	3.9
1	C	393	ASP	3.9
1	D	19	MET	3.9
1	A	554	GLY	3.9
1	B	468	GLY	3.9
1	A	466	PRO	3.9
1	C	233	ASP	3.9
1	A	267	GLU	3.9
1	B	263	LYS	3.9
1	B	501	ILE	3.8
1	D	196	GLY	3.8
1	D	252	LEU	3.8
1	D	339	LEU	3.8
1	B	101	ALA	3.8
1	B	430	GLU	3.8
1	B	460	ASP	3.8
1	A	224	ASP	3.8
1	D	173	THR	3.8
1	D	50	VAL	3.8
1	D	392	LEU	3.8
1	D	180	GLY	3.8
1	A	312	LEU	3.8
1	B	37	PRO	3.8
1	B	139	VAL	3.8
1	D	334	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	514	LYS	3.8
1	B	337	VAL	3.8
1	C	110	MET	3.8
1	B	381	VAL	3.8
1	B	458	ASN	3.8
1	C	354	ALA	3.8
1	A	468	GLY	3.8
1	A	144	ALA	3.7
1	C	266	ALA	3.7
1	D	176	ALA	3.7
1	A	362	ARG	3.7
1	A	434	SER	3.7
1	A	170	ASN	3.7
1	B	51	GLY	3.7
1	C	336	ASP	3.7
1	D	407	VAL	3.7
1	D	143	PRO	3.7
1	C	471	GLN	3.7
1	A	293	PRO	3.7
1	A	221	THR	3.7
1	D	69	ILE	3.7
1	B	74	GLY	3.7
1	B	461	GLY	3.7
1	A	517	ARG	3.7
1	D	444	GLU	3.7
1	D	398	SER	3.7
1	B	6	GLY	3.7
1	B	161	ALA	3.7
1	A	527	ARG	3.7
1	A	309	VAL	3.7
1	C	283	LEU	3.7
1	A	172	PRO	3.7
1	C	114	GLN	3.7
1	D	134	PRO	3.6
1	B	363	LYS	3.6
1	B	498	LYS	3.6
1	C	218	VAL	3.6
1	B	72	LEU	3.6
1	C	282	ASN	3.6
1	D	525	ALA	3.6
1	D	434	SER	3.6
1	D	268	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	451	ASN	3.6
1	C	237	ILE	3.6
1	A	339	LEU	3.6
1	A	361	PRO	3.6
1	C	261	ARG	3.6
1	A	461	GLY	3.6
1	D	27	LEU	3.6
1	A	233	ASP	3.6
1	A	16	VAL	3.6
1	D	343	GLN	3.6
1	B	466	PRO	3.6
1	C	4	ILE	3.6
1	B	386	VAL	3.6
1	D	411	LEU	3.6
1	A	424	GLN	3.5
1	A	407	VAL	3.5
1	A	168	ILE	3.5
1	B	339	LEU	3.5
1	B	221	THR	3.5
1	B	41	ALA	3.5
1	B	138	ALA	3.5
1	C	362	ARG	3.5
1	C	468	GLY	3.5
1	C	71	ARG	3.5
1	A	105	VAL	3.5
1	C	313	VAL	3.5
1	B	119	VAL	3.5
1	B	189	THR	3.5
1	D	154	THR	3.5
1	C	178	ALA	3.5
1	A	132	GLY	3.5
1	C	268	LYS	3.5
1	C	6	GLY	3.5
1	B	234	SER	3.5
1	B	361	PRO	3.5
1	A	464	PRO	3.5
1	A	465	ALA	3.5
1	A	509	GLU	3.5
1	C	280	ASP	3.5
1	A	287	THR	3.5
1	D	618	LEU	3.5
1	C	470	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	394	VAL	3.5
1	D	417	THR	3.5
1	C	351	LYS	3.5
1	C	135	VAL	3.5
1	C	281	VAL	3.5
1	A	230	GLU	3.5
1	D	621	THR	3.5
1	B	357	PHE	3.4
1	B	459	LEU	3.4
1	D	271	ILE	3.4
1	C	296	MET	3.4
1	D	175	ALA	3.4
1	D	70	LYS	3.4
1	C	344	THR	3.4
1	B	314	ASN	3.4
1	B	500	THR	3.4
1	A	330	SER	3.4
1	A	131	LEU	3.4
1	A	179	TYR	3.4
1	D	530	GLU	3.4
1	B	316	SER	3.4
1	B	352	LYS	3.4
1	B	42	TYR	3.4
1	B	52	GLN	3.4
1	A	218	VAL	3.4
1	A	493	SER	3.4
1	C	241	VAL	3.4
1	D	17	ALA	3.4
1	B	451	ASN	3.4
1	A	119	VAL	3.4
1	D	443	GLY	3.4
1	D	131	LEU	3.4
1	C	55	LYS	3.4
1	D	282	ASN	3.4
1	B	453	SER	3.4
1	B	454	LEU	3.4
1	B	69	ILE	3.4
1	C	348	MET	3.3
1	D	390	LEU	3.3
1	D	370	ALA	3.3
1	A	200	PHE	3.3
1	A	116	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	416	THR	3.3
1	B	48	THR	3.3
1	C	392	LEU	3.3
1	A	90	PRO	3.3
1	C	180	GLY	3.3
1	B	231	ASP	3.3
1	A	460	ASP	3.3
1	C	53	PRO	3.3
1	B	111	ALA	3.3
1	D	527	ARG	3.3
1	C	618	LEU	3.3
1	A	126	THR	3.3
1	A	263	LYS	3.3
1	D	409	THR	3.3
1	B	343	GLN	3.3
1	D	228	GLY	3.3
1	A	110	MET	3.3
1	B	507	LEU	3.3
1	A	544	HIS	3.3
1	B	158	GLY	3.3
1	C	39	ILE	3.3
1	B	397	LEU	3.3
1	B	432	ASN	3.3
1	B	63	GLN	3.3
1	A	529	PHE	3.3
1	A	358	GLY	3.3
1	A	36	THR	3.3
1	D	229	GLY	3.3
1	A	91	PHE	3.3
1	B	448	ALA	3.3
1	C	309	VAL	3.3
1	D	129	ASP	3.3
1	A	482	GLY	3.2
1	C	174	ALA	3.2
1	D	9	LEU	3.2
1	A	507	LEU	3.2
1	C	341	GLY	3.2
1	D	396	PRO	3.2
1	C	505	SER	3.2
1	B	472	ILE	3.2
1	D	130	TYR	3.2
1	D	412	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	557	LEU	3.2
1	C	378	GLN	3.2
1	A	180	GLY	3.2
1	D	71	ARG	3.2
1	D	371	VAL	3.2
1	D	199	ALA	3.2
1	C	2	GLY	3.2
1	A	442	GLN	3.2
1	D	255	ASP	3.2
1	C	7	ILE	3.2
1	D	402	GLU	3.2
1	D	524	GLU	3.2
1	A	470	PRO	3.2
1	D	361	PRO	3.2
1	D	399	LEU	3.2
1	C	523	ALA	3.2
1	A	181	LEU	3.2
1	D	397	LEU	3.2
1	B	168	ILE	3.2
1	C	113	PRO	3.2
1	C	493	SER	3.2
1	D	253	ARG	3.2
1	A	603	GLN	3.2
1	C	118	GLU	3.2
1	B	620	LEU	3.1
1	D	506	GLY	3.1
1	A	127	ALA	3.1
1	C	103	VAL	3.1
1	C	239	TYR	3.1
1	C	240	LEU	3.1
1	C	528	LYS	3.1
1	A	528	LYS	3.1
1	D	182	ASP	3.1
1	D	454	LEU	3.1
1	D	536	ARG	3.1
1	B	153	ALA	3.1
1	A	133	GLU	3.1
1	A	452	LYS	3.1
1	A	143	PRO	3.1
1	C	492	ASN	3.1
1	C	93	ILE	3.1
1	B	114	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	454	LEU	3.1
1	B	49	LEU	3.1
1	A	111	ALA	3.1
1	A	417	THR	3.1
1	A	441	LEU	3.1
1	D	502	LYS	3.1
1	A	134	PRO	3.1
1	A	602	ALA	3.1
1	D	56	ARG	3.1
1	D	476	PHE	3.1
1	A	222	ASN	3.1
1	A	504	SER	3.1
1	C	248	GLN	3.1
1	D	262	LEU	3.1
1	B	309	VAL	3.1
1	C	534	GLN	3.0
1	A	356	PHE	3.0
1	C	524	GLU	3.0
1	C	154	THR	3.0
1	C	251	ASP	3.0
1	D	340	VAL	3.0
1	B	266	ALA	3.0
1	C	12	THR	3.0
1	C	617	ARG	3.0
1	C	137	GLU	3.0
1	A	52	GLN	3.0
1	D	52	GLN	3.0
1	D	394	VAL	3.0
1	A	67	PHE	3.0
1	D	373	ILE	3.0
1	A	454	LEU	3.0
1	C	366	ASN	3.0
1	C	238	ASN	3.0
1	C	469	MET	3.0
1	B	524	GLU	3.0
1	C	101	ALA	3.0
1	C	312	LEU	3.0
1	B	312	LEU	2.9
1	B	470	PRO	2.9
1	C	300	VAL	2.9
1	C	363	LYS	2.9
1	D	127	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	144	ALA	2.9
1	B	356	PHE	2.9
1	A	449	ALA	2.9
1	A	204	ILE	2.9
1	C	216	PHE	2.9
1	D	422	HIS	2.9
1	A	228	GLY	2.9
1	C	231	ASP	2.9
1	C	297	ASN	2.9
1	B	120	LEU	2.9
1	A	219	LEU	2.9
1	A	300	VAL	2.9
1	A	232	PHE	2.9
1	A	227	LEU	2.9
1	D	142	VAL	2.9
1	D	90	PRO	2.9
1	A	72	LEU	2.9
1	C	50	VAL	2.9
1	D	515	MET	2.9
1	C	102	TRP	2.9
1	B	383	THR	2.9
1	D	416	THR	2.9
1	C	179	TYR	2.8
1	A	260	GLN	2.8
1	A	450	ASP	2.8
1	D	259	MET	2.8
1	B	442	GLN	2.8
1	C	269	ALA	2.8
1	D	475	THR	2.8
1	A	422	HIS	2.8
1	D	263	LYS	2.8
1	A	145	TYR	2.8
1	A	387	LYS	2.8
1	C	116	SER	2.8
1	A	411	LEU	2.8
1	D	504	SER	2.8
1	B	526	ASP	2.8
1	C	421	LYS	2.8
1	A	70	LYS	2.8
1	B	390	LEU	2.8
1	C	136	THR	2.8
1	A	408	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	387	LYS	2.8
1	B	506	GLY	2.8
1	C	3	LYS	2.8
1	A	112	PRO	2.8
1	A	285	TYR	2.8
1	C	252	LEU	2.8
1	C	436	VAL	2.8
1	A	120	LEU	2.8
1	C	536	ARG	2.8
1	A	332	SER	2.8
1	D	204	ILE	2.8
1	D	330	SER	2.8
1	A	593	GLN	2.8
1	C	119	VAL	2.8
1	B	349	VAL	2.8
1	B	485	HIS	2.7
1	B	505	SER	2.7
1	A	479	ASP	2.7
1	A	481	ASP	2.7
1	D	518	ASP	2.7
1	B	525	ALA	2.7
1	B	103	VAL	2.7
1	A	334	ILE	2.7
1	A	415	ASN	2.7
1	A	423	SER	2.7
1	D	314	ASN	2.7
1	D	179	TYR	2.7
1	B	265	ALA	2.7
1	B	447	ARG	2.7
1	B	382	LEU	2.7
1	A	502	LYS	2.7
1	C	242	GLU	2.7
1	D	88	ILE	2.7
1	A	431	ASP	2.7
1	B	235	ARG	2.7
1	A	123	MET	2.7
1	D	410	THR	2.7
1	B	75	ARG	2.7
1	A	202	ILE	2.7
1	C	22	THR	2.7
1	D	433	GLN	2.7
1	C	286	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	299	LYS	2.7
1	D	619	LEU	2.7
1	D	491	LYS	2.6
1	C	58	ALA	2.6
1	C	343	GLN	2.6
1	D	313	VAL	2.6
1	C	253	ARG	2.6
1	A	360	GLU	2.6
1	A	594	VAL	2.6
1	C	279	THR	2.6
1	D	2	GLY	2.6
1	A	301	THR	2.6
1	B	353	VAL	2.6
1	D	430	GLU	2.6
1	C	464	PRO	2.6
1	A	421	LYS	2.6
1	D	481	ASP	2.6
1	C	259	MET	2.6
1	A	284	PRO	2.6
1	B	484	LEU	2.6
1	A	113	PRO	2.6
1	C	181	LEU	2.6
1	D	181	LEU	2.6
1	B	334	ILE	2.6
1	B	27	LEU	2.6
1	B	438	ILE	2.6
1	B	492	ASN	2.5
1	A	565	ILE	2.5
1	C	172	PRO	2.5
1	B	65	THR	2.5
1	B	465	ALA	2.5
1	A	305	LEU	2.5
1	A	526	ASP	2.5
1	D	426	PHE	2.5
1	C	260	GLN	2.5
1	D	65	THR	2.5
1	A	142	VAL	2.5
1	A	437	THR	2.5
1	D	169	ILE	2.5
1	D	265	ALA	2.5
1	A	14	SER	2.5
1	B	317	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	370	ALA	2.5
1	B	34	ARG	2.5
1	B	162	GLY	2.5
1	D	483	ILE	2.5
1	D	383	THR	2.5
1	A	177	LEU	2.5
1	D	425	VAL	2.5
1	D	198	GLY	2.5
1	D	216	PHE	2.5
1	A	178	ALA	2.5
1	B	93	ILE	2.5
1	C	367	PRO	2.5
1	A	378	GLN	2.5
1	B	3	LYS	2.5
1	D	477	ASP	2.5
1	A	197	GLY	2.5
1	D	51	GLY	2.5
1	D	329	LEU	2.5
1	D	622	GLY	2.5
1	A	108	GLN	2.5
1	C	94	ILE	2.5
1	A	340	VAL	2.5
1	C	463	ASN	2.5
1	B	310	GLU	2.4
1	D	230	GLU	2.4
1	D	507	LEU	2.4
1	C	420	THR	2.4
1	B	509	GLU	2.4
1	D	535	THR	2.4
1	D	254	ASN	2.4
1	B	450	ASP	2.4
1	A	369	GLU	2.4
1	A	534	GLN	2.4
1	B	463	ASN	2.4
1	D	617	ARG	2.4
1	B	90	PRO	2.4
1	D	55	LYS	2.4
1	A	195	LEU	2.4
1	C	503	ALA	2.4
1	A	114	GLN	2.4
1	B	19	MET	2.4
1	A	15	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	335	ASP	2.4
1	B	417	THR	2.4
1	C	244	PHE	2.4
1	D	360	GLU	2.4
1	B	64	ASN	2.4
1	A	182	ASP	2.4
1	C	258	ALA	2.4
1	C	428	THR	2.4
1	B	380	GLY	2.4
1	C	234	SER	2.4
1	A	601	ILE	2.4
1	D	385	ASP	2.4
1	D	466	PRO	2.4
1	D	492	ASN	2.4
1	B	389	VAL	2.4
1	B	367	PRO	2.3
1	B	194	ASP	2.3
1	D	205	ILE	2.3
1	D	395	THR	2.3
1	B	528	LYS	2.3
1	B	215	THR	2.3
1	B	260	GLN	2.3
1	C	308	LEU	2.3
1	A	359	LYS	2.3
1	B	167	ARG	2.3
1	C	402	GLU	2.3
1	A	524	GLU	2.3
1	D	264	GLU	2.3
1	B	366	ASN	2.3
1	C	390	LEU	2.3
1	D	534	GLN	2.3
1	D	167	ARG	2.3
1	D	126	THR	2.3
1	C	25	ARG	2.3
1	C	507	LEU	2.3
1	D	620	LEU	2.3
1	B	177	LEU	2.3
1	A	399	LEU	2.3
1	D	389	VAL	2.3
1	D	31	GLU	2.3
1	A	363	LYS	2.3
1	A	207	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	458	ASN	2.3
1	D	258	ALA	2.3
1	A	59	VAL	2.3
1	A	62	PRO	2.3
1	D	178	ALA	2.2
1	A	81	GLU	2.2
1	A	261	ARG	2.2
1	B	17	ALA	2.2
1	B	519	ALA	2.2
1	C	620	LEU	2.2
1	B	471	GLN	2.2
1	B	262	LEU	2.2
1	D	317	ILE	2.2
1	D	251	ASP	2.2
1	D	116	SER	2.2
1	C	70	LYS	2.2
1	D	447	ARG	2.2
1	A	425	VAL	2.2
1	A	2	GLY	2.2
1	D	448	ALA	2.2
1	D	53	PRO	2.2
1	C	17	ALA	2.2
1	C	23	THR	2.2
1	C	190	ILE	2.2
1	A	400	GLY	2.2
1	D	449	ALA	2.2
1	A	208	ASP	2.2
1	B	449	ALA	2.2
1	D	516	VAL	2.2
1	D	63	GLN	2.2
1	C	301	THR	2.2
1	C	219	LEU	2.2
1	B	16	VAL	2.2
1	D	119	VAL	2.2
1	B	185	THR	2.2
1	A	365	VAL	2.2
1	A	448	ALA	2.2
1	D	189	THR	2.2
1	C	255	ASP	2.2
1	B	100	ASP	2.2
1	C	452	LYS	2.2
1	C	385	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	355	GLU	2.2
1	A	472	ILE	2.2
1	C	386	VAL	2.2
1	C	236	LEU	2.2
1	B	515	MET	2.1
1	C	138	ALA	2.1
1	B	331	VAL	2.1
1	D	64	ASN	2.1
1	A	23	THR	2.1
1	A	97	ASP	2.1
1	D	446	LYS	2.1
1	C	229	GLY	2.1
1	C	109	LYS	2.1
1	B	364	ASP	2.1
1	D	482	GLY	2.1
1	C	519	ALA	2.1
1	B	271	ILE	2.1
1	A	154	THR	2.1
1	D	132	GLY	2.1
1	D	480	ALA	2.1
1	A	64	ASN	2.1
1	C	134	PRO	2.1
1	B	18	ILE	2.1
1	D	3	LYS	2.1
1	A	60	THR	2.1
1	A	229	GLY	2.1
1	D	316	SER	2.1
1	B	102	TRP	2.1
1	D	508	ASN	2.1
1	B	340	VAL	2.1
1	C	20	ASP	2.1
1	A	555	ASP	2.1
1	C	131	LEU	2.1
1	A	313	VAL	2.1
1	C	270	LYS	2.1
1	C	89	MET	2.1
1	B	482	GLY	2.1
1	D	418	ILE	2.1
1	B	59	VAL	2.1
1	C	435	ALA	2.1
1	C	11	THR	2.1
1	D	348	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	115	ILE	2.1
1	A	37	PRO	2.1
1	D	87	SER	2.1
1	D	332	SER	2.1
1	D	511	GLU	2.1
1	C	100	ASP	2.0
1	A	490	ASP	2.0
1	C	466	PRO	2.0
1	A	518	ASP	2.0
1	B	152	GLN	2.0
1	A	175	ALA	2.0
1	A	205	ILE	2.0
1	D	184	GLY	2.0
1	B	362	ARG	2.0
1	D	281	VAL	2.0
1	D	517	ARG	2.0
1	D	7	ILE	2.0
1	B	440	VAL	2.0
1	C	60	THR	2.0
1	B	329	LEU	2.0
1	A	364	ASP	2.0
1	B	123	MET	2.0
1	C	228	GLY	2.0
1	B	188	ARG	2.0
1	B	452	LYS	2.0
1	B	237	ILE	2.0
1	C	619	LEU	2.0
1	B	521	ALA	2.0
1	B	348	MET	2.0
1	A	19	MET	2.0
1	C	622	GLY	2.0
1	D	218	VAL	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 ⓘ

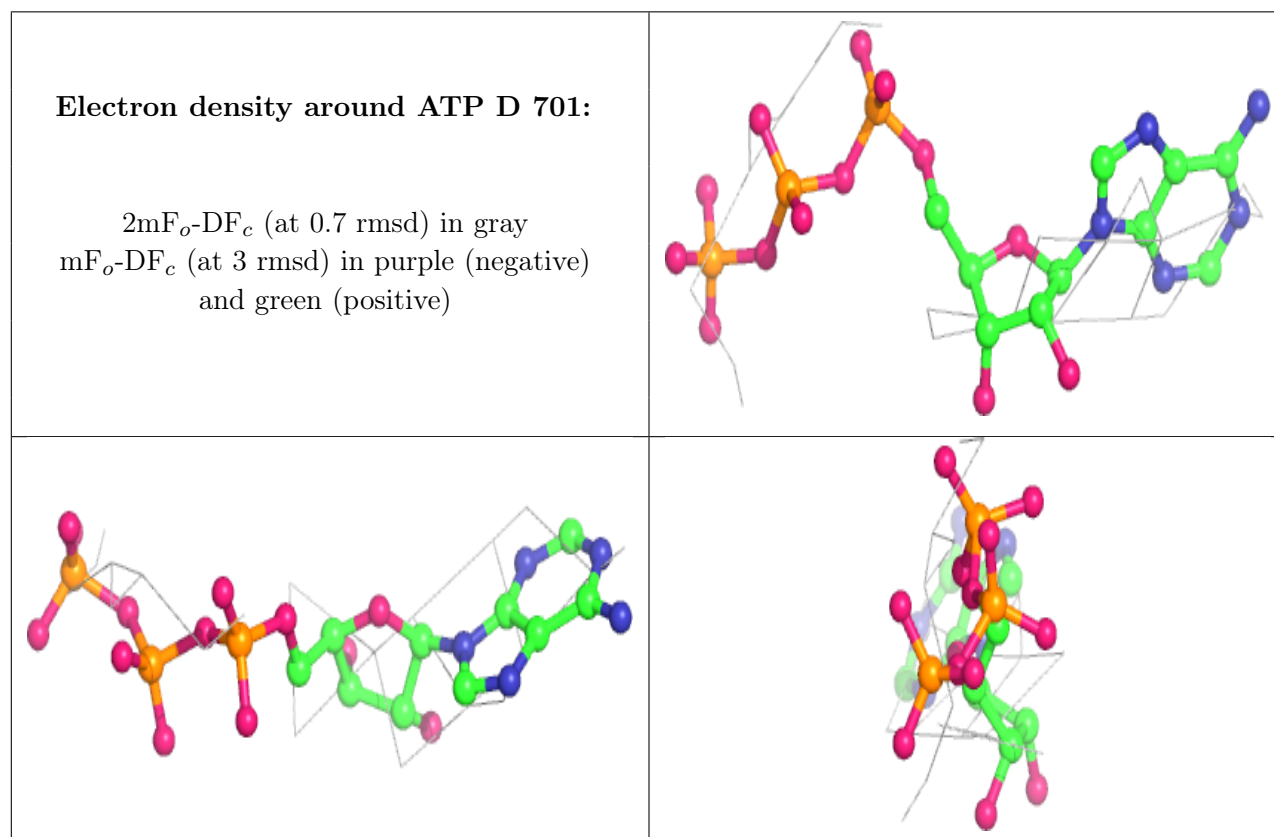
There are no monosaccharides in this entry.

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.

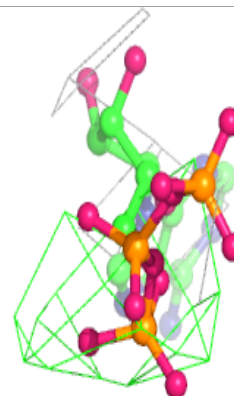
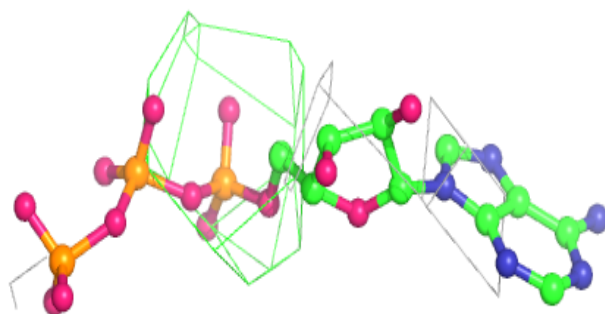
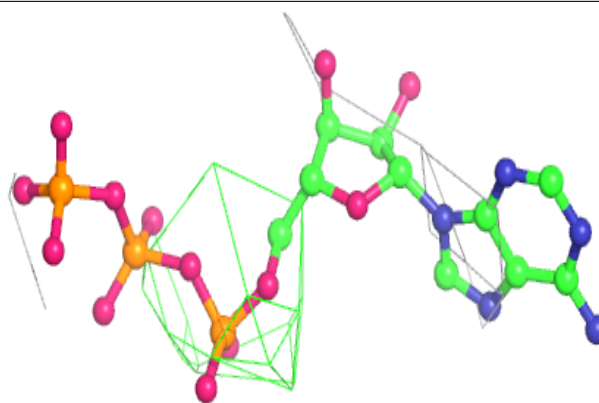
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	D	701	31/31	0.82	0.67	319,319,319,319	0
2	ATP	B	701	31/31	0.85	0.41	319,319,319,319	0
2	ATP	C	701	31/31	0.87	0.46	320,320,320,320	0
2	ATP	A	701	31/31	0.92	0.43	319,319,319,319	0

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.

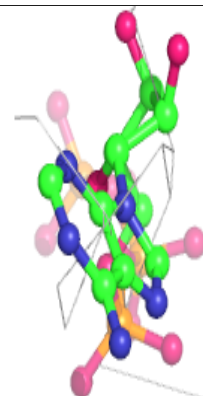
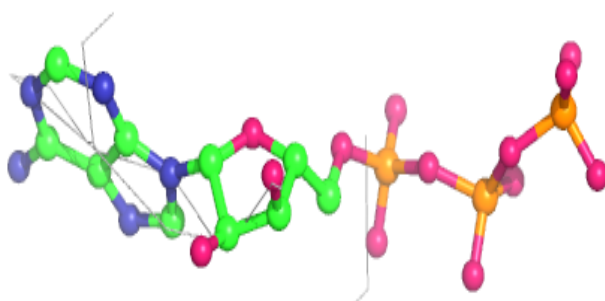
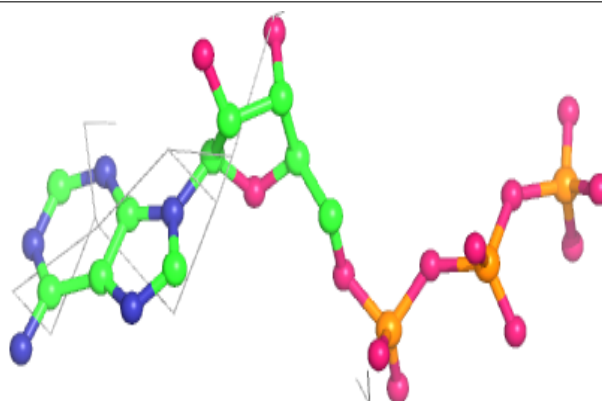


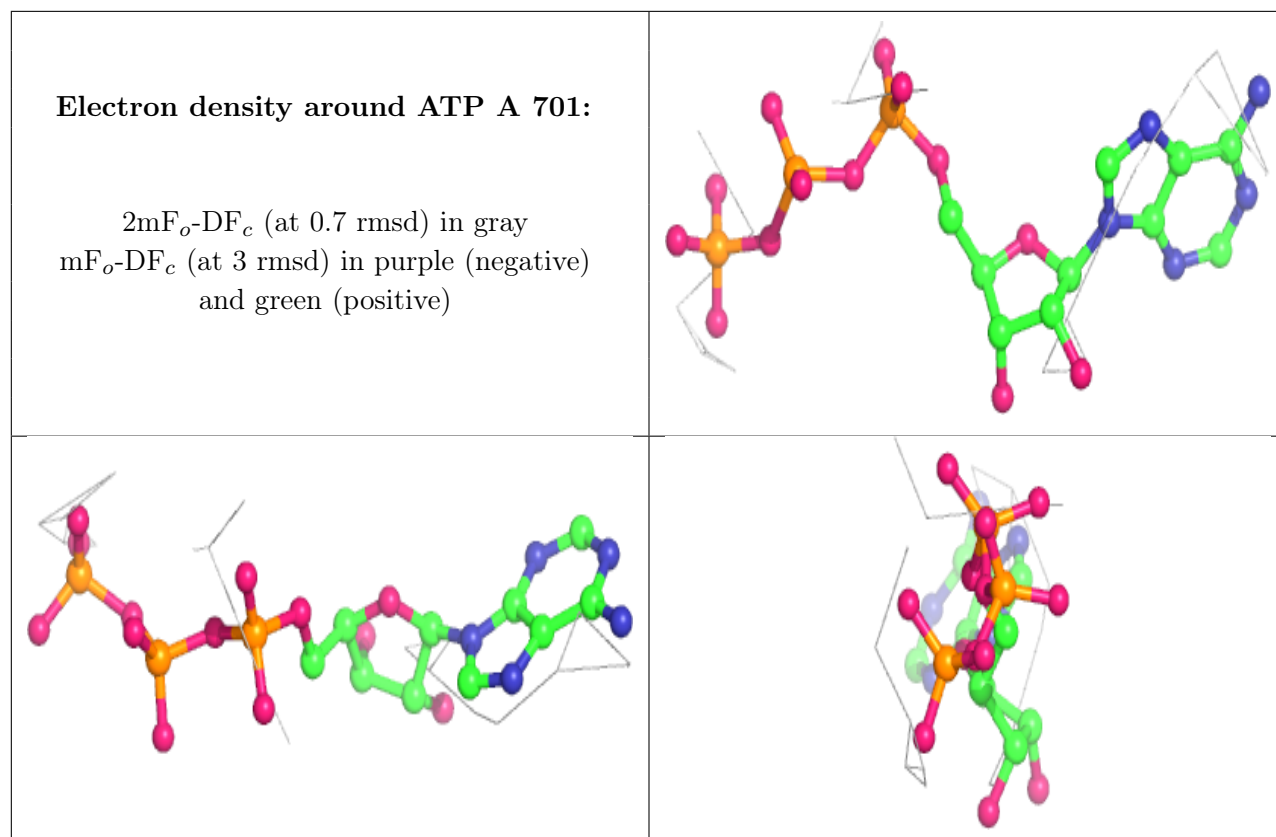
Electron density around ATP B 701:

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

**Electron density around ATP C 701:**

$2mF_o - DF_c$ (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.