



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:17 AM UTC

PDB ID : 7ZBH / pdb_00007zbh
Title : ATP-dependent zinc metalloprotease FtsH (BB0789) from *Borrelia burgdorferi*
Authors : Brangulis, K.
Deposited on : 2022-03-23
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

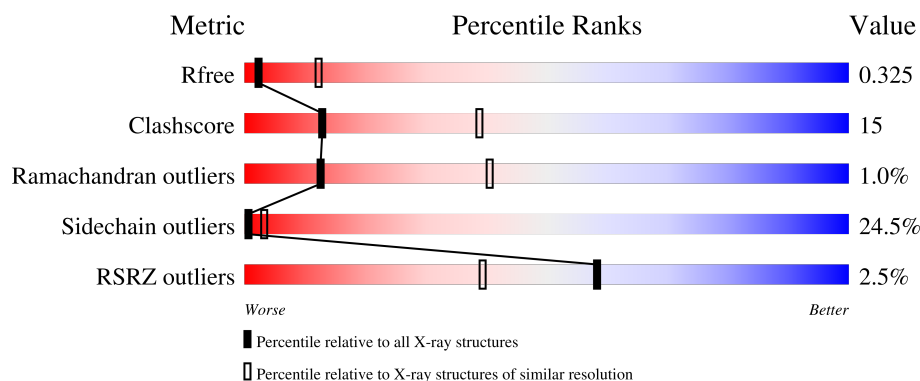
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	453	0.3% 45% 31% 5% 19%
1	B	453	3% 46% 30% 7% 17%
1	D	453	2% 48% 28% 5% 19%
1	F	453	2% 49% 27% 6% 19%
1	I	453	3% 43% 33% . 19%

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Mol	Chain	Length	Quality of chain
1	K	453	2% 46% 30% 6% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16396 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 ATP-dependent zinc metalloprotease FtsH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2703	1722	463	510	8			
1	B	374	Total	C	N	O	S	0	0	0
			2752	1748	473	523	8			
1	D	366	Total	C	N	O	S	0	0	0
			2678	1704	456	510	8			
1	F	367	Total	C	N	O	S	0	0	0
			2692	1712	461	511	8			
1	I	367	Total	C	N	O	S	0	0	0
			2701	1716	466	511	8			
1	K	368	Total	C	N	O	S	0	0	0
			2702	1718	464	512	8			

There are 18 discrepancies between the modelled and reference sequences:

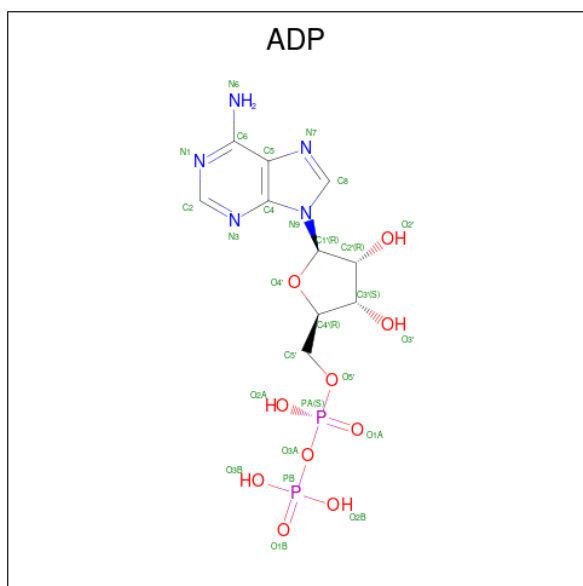
Chain	Residue	Modelled	Actual	Comment	Reference
A	162	GLY	-	expression tag	UNP O51729
A	163	ALA	-	expression tag	UNP O51729
A	164	MET	-	expression tag	UNP O51729
B	162	GLY	-	expression tag	UNP O51729
B	163	ALA	-	expression tag	UNP O51729
B	164	MET	-	expression tag	UNP O51729
D	162	GLY	-	expression tag	UNP O51729
D	163	ALA	-	expression tag	UNP O51729
D	164	MET	-	expression tag	UNP O51729
F	162	GLY	-	expression tag	UNP O51729
F	163	ALA	-	expression tag	UNP O51729
F	164	MET	-	expression tag	UNP O51729
I	162	GLY	-	expression tag	UNP O51729
I	163	ALA	-	expression tag	UNP O51729
I	164	MET	-	expression tag	UNP O51729
K	162	GLY	-	expression tag	UNP O51729
K	163	ALA	-	expression tag	UNP O51729

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Chain	Residue	Modelled	Actual	Comment	Reference
K	164	MET	-	expression tag	UNP O51729

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	27	0
			27	10	5	10	2		

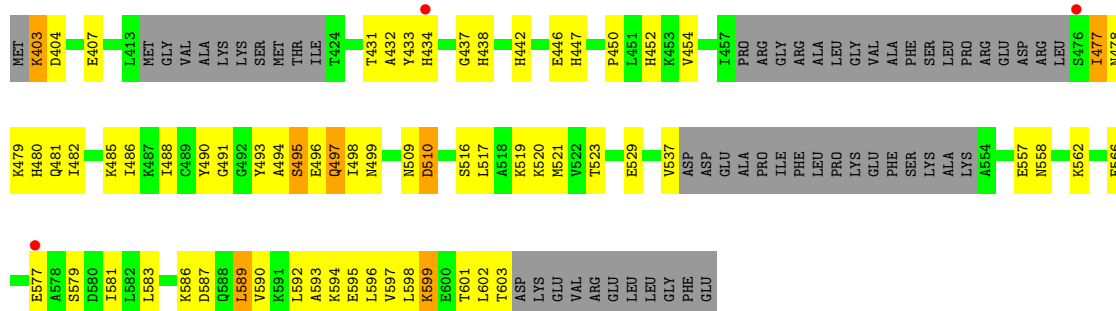
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

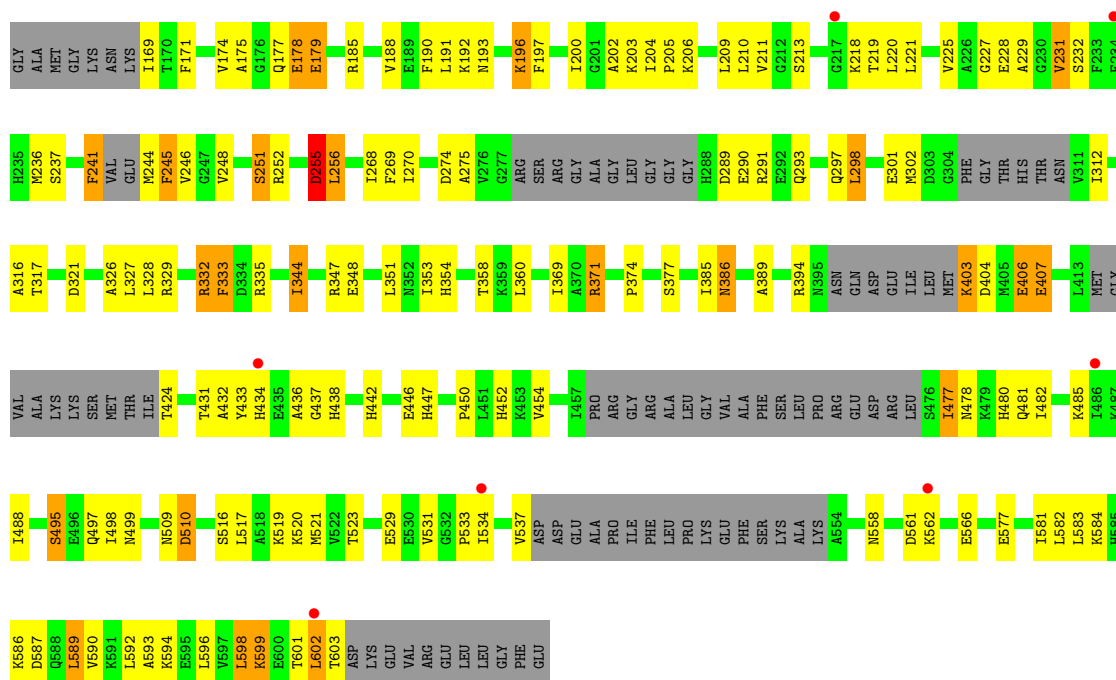
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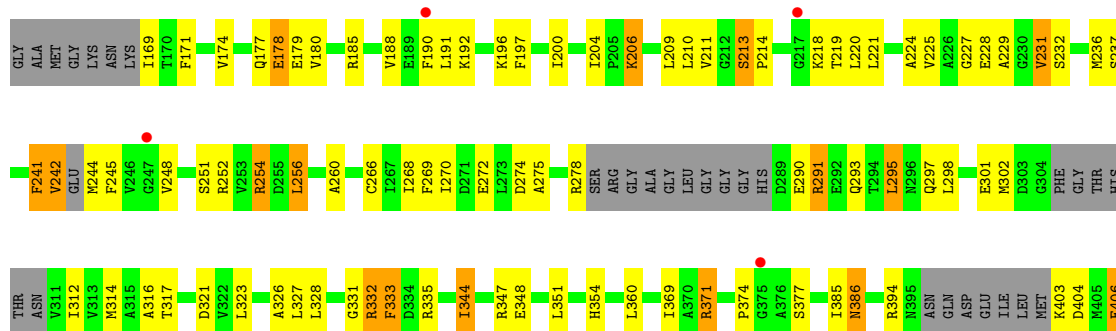
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Zn 1	1	0
3	I	1	Total 1	Zn 1	1	0
3	K	1	Total 1	Zn 1	1	0

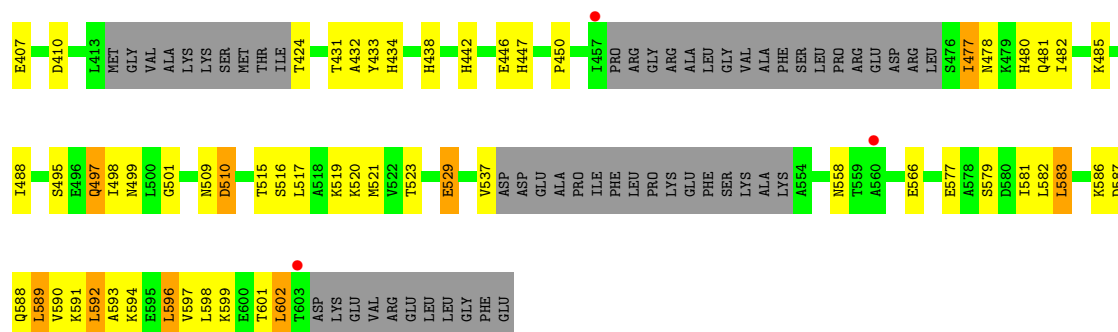


● Molecule 1: ATP-dependent zinc metalloprotease FtsH

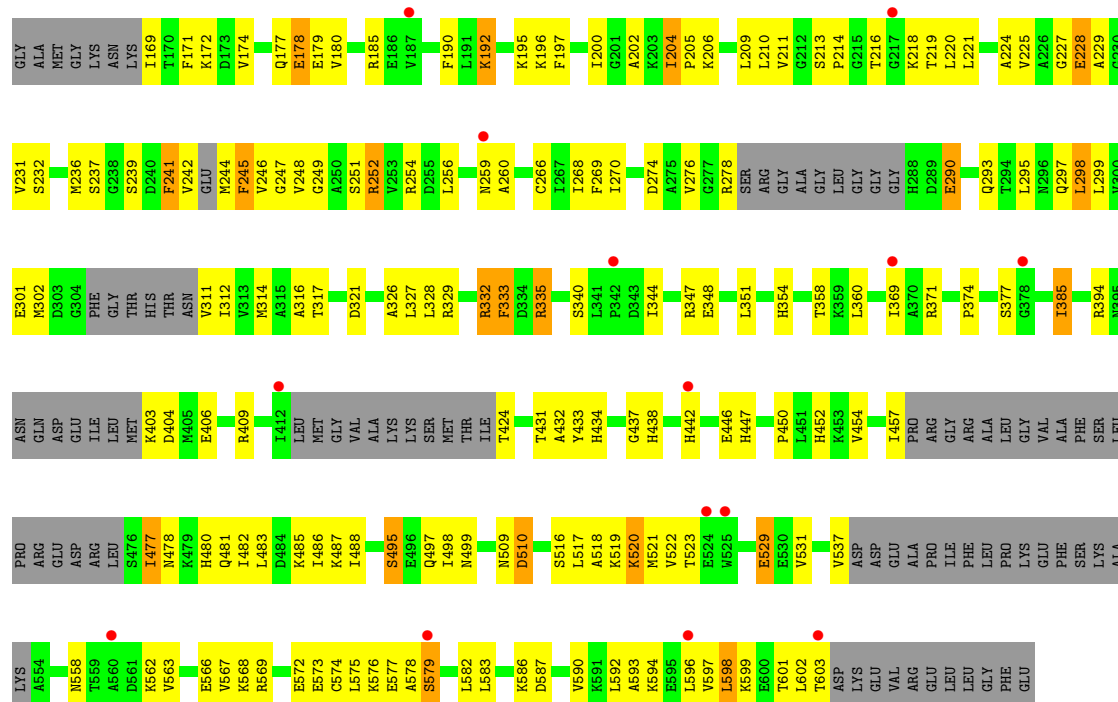
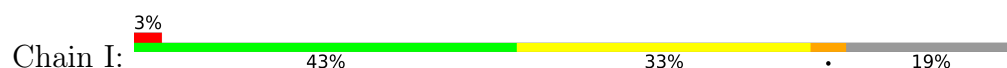


● Molecule 1: ATP-dependent zinc metalloprotease FtsH

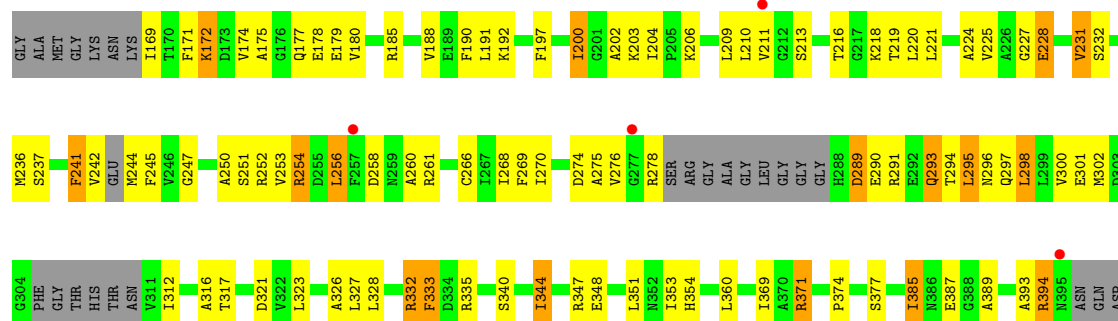


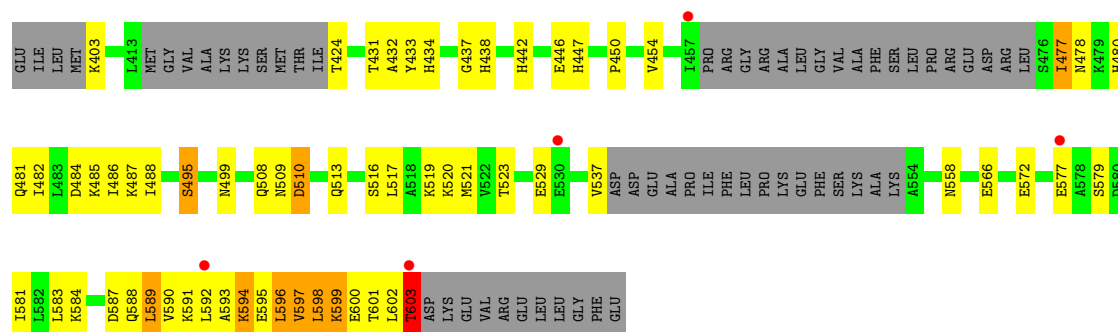


• Molecule 1: ATP-dependent zinc metalloprotease FtsH



• Molecule 1: ATP-dependent zinc metalloprotease FtsH





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.81Å 192.80Å 114.13Å 90.00° 124.31° 90.00°	Depositor
Resolution (Å)	96.75 – 3.30 96.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (96.75-3.30) 97.8 (96.75-3.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.279 , 0.332 0.279 , 0.325	Depositor DCC
R_{free} test set	2048 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 144.6	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	0.91	EDS
Total number of atoms	16396	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.13	0/2736	1.68	8/3687 (0.2%)
1	B	1.12	0/2786	1.68	3/3755 (0.1%)
1	D	1.12	1/2709 (0.0%)	1.71	5/3650 (0.1%)
1	F	1.13	0/2722	1.69	2/3666 (0.1%)
1	I	1.16	2/2732 (0.1%)	1.67	2/3679 (0.1%)
1	K	1.14	2/2733 (0.1%)	1.67	4/3681 (0.1%)
All	All	1.13	5/16418 (0.0%)	1.68	24/22118 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	452	HIS	CG-CD2	10.14	1.47	1.35
1	I	452	HIS	ND1-CE1	8.61	1.41	1.32
1	D	534	ILE	C-O	5.69	1.29	1.24
1	K	572	GLU	CD-OE2	5.54	1.35	1.25
1	K	508	GLN	CD-NE2	5.08	1.44	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	ASP	CA-CB-CG	6.80	119.40	112.60
1	D	510	ASP	CA-CB-CG	6.59	119.19	112.60
1	K	510	ASP	CA-CB-CG	6.54	119.14	112.60
1	D	255	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	493	TYR	N-CA-C	-6.46	104.32	111.82
1	F	510	ASP	CA-CB-CG	6.21	118.81	112.60
1	I	510	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	510	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	255	ASP	CA-CB-CG	5.91	118.50	112.60
1	A	289	ASP	CA-C-N	5.56	128.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ASP	C-N-CA	5.56	128.29	120.28
1	K	603	THR	CA-C-O	5.40	129.98	120.80
1	A	457	ILE	CB-CA-C	5.36	116.94	110.78
1	B	433	TYR	CA-C-O	-5.30	115.24	120.70
1	A	433	TYR	CA-C-O	-5.30	115.24	120.70
1	K	597	VAL	N-CA-C	-5.23	106.11	112.76
1	F	433	TYR	CA-C-O	-5.21	115.33	120.70
1	I	433	TYR	CA-C-O	-5.17	115.38	120.70
1	D	433	TYR	CA-C-O	-5.15	115.39	120.70
1	D	436	ALA	CA-C-N	5.10	125.60	119.94
1	D	436	ALA	C-N-CA	5.10	125.60	119.94
1	K	433	TYR	CA-C-O	-5.06	115.49	120.70
1	A	436	ALA	CA-C-N	5.02	125.51	119.94
1	A	436	ALA	C-N-CA	5.02	125.51	119.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2703	0	2588	79	0
1	B	2752	0	2631	93	0
1	D	2678	0	2556	80	0
1	F	2692	0	2582	74	0
1	I	2701	0	2594	78	0
1	K	2702	0	2589	93	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	D	27	0	12	0	0
2	F	27	0	12	0	0
2	I	27	0	12	0	0
2	K	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
All	All	16396	0	15612	479	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 15.

All (479) 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:403:LYS:O	1:D:406:GLU:CD	1.92	1.11
1:B:305:PHE:HB3	1:B:307:THR:HG23	1.62	0.82
1:A:599:LYS:HD3	1:A:602:LEU:HB2	1.61	0.82
1:D:403:LYS:O	1:D:406:GLU:OE2	1.98	0.82
1:K:599:LYS:HD3	1:K:602:LEU:HB2	1.64	0.80
1:I:190:PHE:CD1	1:I:204:ILE:HG21	2.19	0.77
1:D:244:MET:O	1:D:290:GLU:OE2	2.04	0.76
1:A:437:GLY:HA3	1:A:491:GLY:O	1.86	0.76
1:F:438:HIS:CE1	1:F:510:ASP:OD2	2.40	0.74
1:I:438:HIS:CE1	1:I:510:ASP:OD2	2.41	0.72
1:A:387:GLU:OE2	1:B:335:ARG:NH2	2.22	0.72
1:I:438:HIS:NE2	1:I:510:ASP:OD2	2.23	0.72
1:D:406:GLU:N	1:D:406:GLU:OE1	2.23	0.72
1:D:438:HIS:CE1	1:D:510:ASP:OD2	2.42	0.72
1:F:438:HIS:NE2	1:F:510:ASP:OD2	2.23	0.71
1:A:241:PHE:HZ	1:A:256:LEU:HD22	1.53	0.71
1:K:438:HIS:CE1	1:K:510:ASP:OD2	2.43	0.71
1:K:438:HIS:NE2	1:K:510:ASP:OD2	2.23	0.70
1:A:499:ASN:HD21	1:A:589:LEU:HD21	1.56	0.70
1:B:302:MET:C	1:B:304:GLY:H	1.98	0.70
1:K:291:ARG:HA	1:K:294:THR:HB	1.73	0.70
1:F:592:LEU:HD11	1:F:602:LEU:HD11	1.73	0.69
1:K:293:GLN:HG2	1:K:294:THR:N	2.07	0.69
1:K:477:ILE:HG22	1:K:481:GLN:HB2	1.75	0.69
1:F:206:LYS:NZ	1:F:332:ARG:HG3	2.08	0.69
1:I:477:ILE:HG22	1:I:481:GLN:HB2	1.75	0.69
1:I:195:LYS:CG	1:I:196:LYS:NZ	2.56	0.68
1:D:244:MET:HB3	1:D:248:VAL:HB	1.75	0.68
1:K:434:HIS:NE2	1:K:438:HIS:NE2	2.42	0.68
1:I:202:ALA:HB2	1:K:389:ALA:HB1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:HA	1:B:200:ILE:O	1.93	0.67
1:D:245:PHE:CD2	1:D:246:VAL:HG12	2.30	0.67
1:B:477:ILE:HG22	1:B:481:GLN:HB2	1.77	0.67
1:D:477:ILE:HG22	1:D:481:GLN:HB2	1.78	0.66
1:F:206:LYS:HZ1	1:F:332:ARG:HG3	1.61	0.66
1:B:244:MET:HB3	1:B:248:VAL:HB	1.78	0.65
1:I:244:MET:HB3	1:I:248:VAL:HB	1.79	0.65
1:A:244:MET:HB3	1:A:248:VAL:HB	1.77	0.65
1:F:477:ILE:HG22	1:F:481:GLN:HB2	1.79	0.65
1:B:209:LEU:HD11	1:B:317:THR:HG22	1.79	0.64
1:F:218:LYS:HE2	1:F:316:ALA:HB1	1.79	0.64
1:K:290:GLU:HA	1:K:293:GLN:CD	2.23	0.64
1:F:434:HIS:NE2	1:F:438:HIS:NE2	2.43	0.64
1:F:209:LEU:HD11	1:F:317:THR:HG22	1.80	0.64
1:K:209:LEU:HD11	1:K:317:THR:HG22	1.80	0.63
1:A:477:ILE:HG22	1:A:481:GLN:HB2	1.80	0.63
1:I:209:LEU:HD11	1:I:317:THR:HG22	1.79	0.63
1:B:386:ASN:HD21	1:D:203:LYS:HG2	1.64	0.63
1:F:499:ASN:HD21	1:F:589:LEU:HD21	1.63	0.63
1:D:245:PHE:CE2	1:D:246:VAL:HG12	2.34	0.62
1:B:296:ASN:O	1:B:300:VAL:HG23	1.99	0.62
1:B:303:ASP:O	1:B:304:GLY:C	2.42	0.62
1:D:193:ASN:CG	1:D:196:LYS:HD2	2.25	0.62
1:K:499:ASN:HD21	1:K:589:LEU:HD21	1.65	0.62
1:B:499:ASN:HD21	1:B:589:LEU:HD21	1.64	0.62
1:B:495:SER:HB3	1:B:589:LEU:HD11	1.81	0.61
1:D:218:LYS:HE2	1:D:316:ALA:HB1	1.83	0.61
1:D:326:ALA:O	1:D:332:ARG:NH1	2.34	0.61
1:I:434:HIS:NE2	1:I:438:HIS:NE2	2.43	0.61
1:A:209:LEU:HD11	1:A:317:THR:HG22	1.83	0.61
1:B:302:MET:C	1:B:304:GLY:N	2.59	0.60
1:A:386:ASN:HD21	1:B:203:LYS:HG2	1.65	0.60
1:D:598:LEU:HG	1:D:599:LYS:N	2.16	0.60
1:D:209:LEU:HD11	1:D:317:THR:HG22	1.82	0.60
1:D:602:LEU:HG	1:D:603:THR:N	2.15	0.60
1:B:304:GLY:O	1:B:305:PHE:HB2	2.02	0.60
1:I:195:LYS:CG	1:I:196:LYS:HZ2	2.15	0.60
1:B:298:LEU:O	1:B:302:MET:HG2	2.01	0.59
1:B:595:GLU:HA	1:B:598:LEU:HD12	1.83	0.59
1:B:297:GLN:HE21	1:B:301:GLU:HG2	1.68	0.59
1:D:403:LYS:O	1:D:406:GLU:OE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:484:ASP:HA	1:K:487:LYS:HD2	1.83	0.59
1:D:177:GLN:O	1:D:178:GLU:C	2.45	0.59
1:D:358:THR:HA	1:K:200:ILE:O	2.03	0.59
1:A:347:ARG:CZ	1:A:374:PRO:HA	2.33	0.59
1:F:347:ARG:CZ	1:F:374:PRO:HA	2.33	0.58
1:I:566:GLU:O	1:I:569:ARG:HB3	2.04	0.58
1:K:347:ARG:CZ	1:K:374:PRO:HA	2.33	0.58
1:A:484:ASP:O	1:A:488:ILE:HG13	2.03	0.58
1:I:406:GLU:O	1:I:409:ARG:HB3	2.03	0.58
1:K:295:LEU:O	1:K:296:ASN:C	2.45	0.58
1:B:347:ARG:CZ	1:B:374:PRO:HA	2.34	0.58
1:D:175:ALA:HB2	1:D:353:ILE:HD11	1.85	0.58
1:I:598:LEU:HG	1:I:599:LYS:N	2.19	0.58
1:D:499:ASN:HD21	1:D:589:LEU:HD21	1.69	0.58
1:I:347:ARG:CZ	1:I:374:PRO:HA	2.33	0.58
1:B:264:SER:OG	1:B:310:ASN:HB3	2.03	0.58
1:B:495:SER:O	1:B:499:ASN:ND2	2.34	0.58
1:I:247:GLY:N	1:I:290:GLU:OE1	2.36	0.58
1:D:347:ARG:CZ	1:D:374:PRO:HA	2.33	0.57
1:I:299:LEU:HD22	1:I:332:ARG:NH1	2.17	0.57
1:K:256:LEU:HD21	1:K:268:ILE:HG21	1.84	0.57
1:A:389:ALA:HB1	1:B:202:ALA:HB2	1.85	0.57
1:A:169:ILE:O	1:A:227:GLY:HA3	2.05	0.57
1:B:432:ALA:HB1	1:B:593:ALA:HA	1.86	0.57
1:B:305:PHE:HB3	1:B:307:THR:CG2	2.33	0.57
1:B:294:THR:O	1:B:297:GLN:HB3	2.05	0.56
1:F:206:LYS:HE2	1:F:331:GLY:C	2.29	0.56
1:F:169:ILE:O	1:F:227:GLY:HA3	2.06	0.56
1:F:326:ALA:O	1:F:332:ARG:NH1	2.38	0.56
1:A:497:GLN:O	1:A:498:ILE:C	2.46	0.56
1:I:169:ILE:O	1:I:227:GLY:HA3	2.06	0.56
1:I:576:LYS:O	1:I:577:GLU:C	2.48	0.56
1:D:495:SER:O	1:D:499:ASN:ND2	2.39	0.56
1:B:599:LYS:C	1:B:601:THR:H	2.14	0.56
1:B:190:PHE:HA	1:B:197:PHE:CE2	2.41	0.55
1:I:568:LYS:O	1:I:572:GLU:HG3	2.06	0.55
1:F:495:SER:O	1:F:499:ASN:ND2	2.39	0.55
1:B:169:ILE:O	1:B:227:GLY:HA3	2.06	0.55
1:B:298:LEU:O	1:B:298:LEU:HD12	2.07	0.55
1:D:169:ILE:O	1:D:227:GLY:HA3	2.06	0.55
1:K:290:GLU:HG3	1:K:294:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:PHE:HA	1:I:197:PHE:CE2	2.40	0.55
1:I:516:SER:O	1:I:520:LYS:HG3	2.07	0.55
1:A:193:ASN:HB3	1:A:196:LYS:HD2	1.88	0.55
1:D:561:ASP:OD2	1:K:558:ASN:OD1	2.25	0.54
1:I:599:LYS:C	1:I:601:THR:H	2.14	0.54
1:K:190:PHE:HA	1:K:197:PHE:CE2	2.42	0.54
1:F:256:LEU:HD21	1:F:268:ILE:HG21	1.90	0.54
1:K:169:ILE:O	1:K:227:GLY:HA3	2.07	0.54
1:D:386:ASN:HD21	1:K:203:LYS:HG2	1.73	0.54
1:A:595:GLU:O	1:A:599:LYS:HG2	2.07	0.53
1:D:406:GLU:OE1	1:D:407:GLU:N	2.39	0.53
1:A:494:ALA:O	1:A:496:GLU:N	2.41	0.53
1:D:599:LYS:C	1:D:601:THR:H	2.17	0.53
1:I:249:GLY:HA2	1:I:252:ARG:HG3	1.89	0.53
1:K:247:GLY:H	1:K:293:GLN:NE2	2.06	0.53
1:A:497:GLN:HG3	1:A:501:GLY:C	2.34	0.53
1:I:434:HIS:CE1	1:I:510:ASP:OD1	2.62	0.53
1:K:434:HIS:CE1	1:K:510:ASP:OD1	2.62	0.53
1:A:599:LYS:C	1:A:601:THR:H	2.16	0.53
1:D:404:ASP:O	1:D:407:GLU:HG2	2.09	0.53
1:F:434:HIS:CE1	1:F:510:ASP:OD1	2.62	0.53
1:D:434:HIS:CE1	1:D:510:ASP:OD1	2.62	0.53
1:A:516:SER:O	1:A:520:LYS:HG3	2.08	0.53
1:K:247:GLY:H	1:K:293:GLN:HE21	1.55	0.53
1:F:241:PHE:O	1:F:244:MET:N	2.42	0.52
1:A:299:LEU:HD22	1:A:332:ARG:NH2	2.24	0.52
1:B:434:HIS:CE1	1:B:510:ASP:OD1	2.63	0.52
1:A:256:LEU:HD21	1:A:268:ILE:HG21	1.90	0.52
1:A:326:ALA:O	1:A:332:ARG:NH1	2.43	0.52
1:F:434:HIS:CD2	1:F:438:HIS:CD2	2.98	0.52
1:B:354:HIS:HB2	1:B:385:ILE:HD12	1.92	0.51
1:F:354:HIS:HB2	1:F:385:ILE:HD12	1.92	0.51
1:K:593:ALA:O	1:K:597:VAL:HG23	2.10	0.51
1:K:290:GLU:HA	1:K:293:GLN:NE2	2.25	0.51
1:K:326:ALA:O	1:K:332:ARG:NH1	2.42	0.51
1:B:256:LEU:HD21	1:B:268:ILE:HG21	1.92	0.51
1:I:442:HIS:HB3	1:I:450:PRO:HA	1.92	0.51
1:A:387:GLU:OE1	1:B:335:ARG:NH1	2.43	0.51
1:K:190:PHE:CD1	1:K:204:ILE:HG12	2.46	0.51
1:I:326:ALA:O	1:I:332:ARG:NH1	2.43	0.51
1:K:495:SER:O	1:K:499:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:602:LEU:HG	1:K:603:THR:N	2.25	0.51
1:I:434:HIS:CD2	1:I:438:HIS:CD2	2.99	0.51
1:K:434:HIS:CD2	1:K:438:HIS:CD2	2.98	0.51
1:F:190:PHE:HA	1:F:197:PHE:CE1	2.46	0.51
1:F:298:LEU:O	1:F:302:MET:HG3	2.11	0.50
1:A:478:ASN:O	1:A:482:ILE:HG12	2.11	0.50
1:B:493:TYR:HE2	1:D:533:PRO:HB3	1.77	0.50
1:B:389:ALA:HB1	1:D:202:ALA:HB2	1.93	0.50
1:D:297:GLN:HE21	1:D:301:GLU:HG2	1.77	0.50
1:F:478:ASN:O	1:F:482:ILE:HG12	2.12	0.50
1:B:434:HIS:CD2	1:B:438:HIS:CD2	2.99	0.50
1:A:602:LEU:HG	1:A:603:THR:N	2.26	0.50
1:B:190:PHE:CD1	1:B:204:ILE:HG12	2.47	0.50
1:D:434:HIS:CD2	1:D:438:HIS:CD2	2.99	0.50
1:K:241:PHE:O	1:K:244:MET:HB2	2.11	0.50
1:A:494:ALA:C	1:A:496:GLU:H	2.20	0.49
1:D:256:LEU:HD21	1:D:268:ILE:HG21	1.94	0.49
1:I:245:PHE:HB3	1:I:248:VAL:HG21	1.93	0.49
1:A:497:GLN:HG3	1:A:501:GLY:O	2.11	0.49
1:A:557:GLU:OE2	1:B:557:GLU:N	2.40	0.49
1:D:190:PHE:CD1	1:D:204:ILE:HG12	2.48	0.49
1:D:447:HIS:CE1	1:D:480:HIS:HB3	2.47	0.49
1:I:213:SER:HB3	1:I:214:PRO:HD2	1.94	0.49
1:D:290:GLU:O	1:D:290:GLU:HG2	2.12	0.49
1:B:437:GLY:HA3	1:B:495:SER:OG	2.13	0.49
1:K:254:ARG:CZ	1:K:254:ARG:HB2	2.42	0.49
1:K:596:LEU:C	1:K:598:LEU:N	2.68	0.49
1:A:534:ILE:HG13	1:F:515:THR:HG23	1.94	0.49
1:B:265:PRO:HA	1:B:310:ASN:O	2.13	0.49
1:D:602:LEU:HG	1:D:603:THR:H	1.77	0.49
1:A:593:ALA:O	1:A:597:VAL:HG23	2.13	0.48
1:B:478:ASN:O	1:B:482:ILE:HG12	2.12	0.48
1:D:478:ASN:O	1:D:482:ILE:HG12	2.13	0.48
1:K:434:HIS:CD2	1:K:438:HIS:NE2	2.81	0.48
1:A:190:PHE:HA	1:A:197:PHE:CE1	2.48	0.48
1:I:478:ASN:O	1:I:482:ILE:HG12	2.13	0.48
1:K:447:HIS:CE1	1:K:480:HIS:HB3	2.48	0.48
1:K:291:ARG:O	1:K:295:LEU:HB3	2.13	0.48
1:B:403:LYS:HD2	1:B:403:LYS:N	2.28	0.48
1:I:437:GLY:HA3	1:I:495:SER:OG	2.13	0.48
1:K:188:VAL:HG12	1:K:192:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:HIS:HB2	1:A:385:ILE:HD12	1.95	0.48
1:A:296:ASN:HA	1:A:299:LEU:HD12	1.94	0.48
1:D:437:GLY:HA3	1:D:495:SER:OG	2.13	0.48
1:I:432:ALA:HB1	1:I:593:ALA:HA	1.94	0.48
1:I:586:LYS:O	1:I:590:VAL:HG23	2.14	0.48
1:K:298:LEU:O	1:K:302:MET:HG3	2.12	0.48
1:D:389:ALA:HB1	1:K:202:ALA:HB2	1.95	0.48
1:D:599:LYS:HE3	1:D:599:LYS:HB3	1.63	0.48
1:K:295:LEU:O	1:K:298:LEU:N	2.47	0.48
1:K:296:ASN:O	1:K:300:VAL:HG23	2.14	0.48
1:K:590:VAL:O	1:K:594:LYS:HE3	2.14	0.48
1:K:595:GLU:O	1:K:599:LYS:HG2	2.13	0.48
1:B:302:MET:O	1:B:304:GLY:N	2.47	0.48
1:D:354:HIS:HB2	1:D:385:ILE:HD12	1.94	0.48
1:F:236:MET:O	1:F:270:ILE:HA	2.14	0.48
1:K:432:ALA:HB1	1:K:593:ALA:HA	1.95	0.48
1:F:593:ALA:O	1:F:597:VAL:HG23	2.14	0.48
1:K:478:ASN:O	1:K:482:ILE:HG12	2.13	0.48
1:I:531:VAL:HG23	1:I:566:GLU:HG3	1.94	0.47
1:K:485:LYS:HA	1:K:488:ILE:HD12	1.96	0.47
1:A:190:PHE:CD1	1:A:204:ILE:HG12	2.48	0.47
1:A:177:GLN:O	1:A:180:VAL:N	2.47	0.47
1:B:442:HIS:HB3	1:B:450:PRO:HA	1.97	0.47
1:D:485:LYS:HA	1:D:488:ILE:HD12	1.96	0.47
1:B:255:ASP:O	1:B:259:ASN:OD1	2.32	0.47
1:I:177:GLN:O	1:I:180:VAL:N	2.48	0.47
1:I:354:HIS:HB2	1:I:385:ILE:HD12	1.96	0.47
1:B:295:LEU:O	1:B:296:ASN:C	2.57	0.47
1:I:578:ALA:O	1:I:579:SER:C	2.58	0.47
1:A:236:MET:O	1:A:270:ILE:HA	2.14	0.47
1:B:485:LYS:HA	1:B:488:ILE:HD12	1.95	0.47
1:B:497:GLN:O	1:B:498:ILE:C	2.58	0.47
1:F:344:ILE:HD13	1:F:371:ARG:HB3	1.97	0.47
1:F:434:HIS:CD2	1:F:438:HIS:NE2	2.83	0.47
1:F:599:LYS:C	1:F:601:THR:H	2.22	0.47
1:K:437:GLY:HA3	1:K:495:SER:OG	2.15	0.47
1:F:447:HIS:CE1	1:F:480:HIS:HB3	2.50	0.47
1:B:447:HIS:CE1	1:B:480:HIS:HB3	2.50	0.47
1:I:434:HIS:CD2	1:I:438:HIS:NE2	2.83	0.47
1:K:236:MET:O	1:K:270:ILE:HA	2.13	0.47
1:B:437:GLY:HA3	1:B:495:SER:HG	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:MET:HE2	1:K:302:MET:HB3	1.81	0.47
1:A:583:LEU:HD13	1:A:583:LEU:HA	1.82	0.46
1:B:190:PHE:CD1	1:B:204:ILE:HG21	2.49	0.46
1:B:236:MET:O	1:B:270:ILE:HA	2.14	0.46
1:B:479:LYS:HG3	1:B:521:MET:HE3	1.97	0.46
1:K:595:GLU:CG	1:K:599:LYS:HD2	2.45	0.46
1:K:596:LEU:C	1:K:598:LEU:H	2.23	0.46
1:B:344:ILE:HD13	1:B:371:ARG:HB3	1.97	0.46
1:F:177:GLN:O	1:F:180:VAL:N	2.48	0.46
1:F:442:HIS:HB3	1:F:450:PRO:HA	1.98	0.46
1:F:485:LYS:HA	1:F:488:ILE:HD12	1.97	0.46
1:K:599:LYS:C	1:K:601:THR:H	2.22	0.46
1:D:236:MET:O	1:D:270:ILE:HA	2.15	0.46
1:K:177:GLN:O	1:K:180:VAL:N	2.48	0.46
1:B:177:GLN:O	1:B:180:VAL:N	2.48	0.46
1:B:296:ASN:HA	1:B:299:LEU:HD12	1.97	0.46
1:B:593:ALA:O	1:B:597:VAL:HG23	2.14	0.46
1:D:432:ALA:HB1	1:D:593:ALA:HA	1.97	0.46
1:F:171:PHE:HD1	1:F:224:ALA:HB1	1.81	0.46
1:I:593:ALA:O	1:I:597:VAL:HG23	2.15	0.46
1:K:219:THR:HG23	1:K:269:PHE:CE2	2.50	0.46
1:K:297:GLN:HE21	1:K:301:GLU:HG2	1.80	0.46
1:K:588:GLN:O	1:K:591:LYS:HB2	2.14	0.46
1:K:442:HIS:HB3	1:K:450:PRO:HA	1.97	0.46
1:D:298:LEU:O	1:D:302:MET:HG3	2.16	0.46
1:I:216:THR:OG1	1:I:218:LYS:HE2	2.15	0.46
1:A:216:THR:OG1	1:A:218:LYS:HE2	2.15	0.46
1:B:216:THR:OG1	1:B:218:LYS:HE2	2.16	0.46
1:B:295:LEU:O	1:B:299:LEU:HG	2.14	0.46
1:B:586:LYS:O	1:B:590:VAL:HG23	2.15	0.46
1:F:516:SER:O	1:F:520:LYS:HG3	2.15	0.46
1:I:335:ARG:NH1	1:K:387:GLU:OE1	2.49	0.46
1:K:216:THR:OG1	1:K:218:LYS:HE2	2.15	0.46
1:A:188:VAL:HG13	1:A:229:ALA:HB2	1.96	0.46
1:D:219:THR:HG23	1:D:269:PHE:CE2	2.49	0.46
1:K:599:LYS:CD	1:K:602:LEU:HB2	2.42	0.46
1:B:178:GLU:OE2	1:B:178:GLU:HA	2.16	0.46
1:B:206:LYS:HD2	1:B:302:MET:O	2.16	0.46
1:I:204:ILE:HG22	1:I:205:PRO:HD2	1.98	0.46
1:K:172:LYS:NZ	1:K:228:GLU:OE2	2.42	0.46
1:F:297:GLN:HE21	1:F:301:GLU:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:297:GLN:HE21	1:I:301:GLU:HG2	1.81	0.46
1:A:327:LEU:O	1:A:333:PHE:HB2	2.16	0.45
1:A:203:LYS:HG2	1:F:386:ASN:HD21	1.80	0.45
1:K:495:SER:HB3	1:K:589:LEU:HD11	1.99	0.45
1:A:247:GLY:N	1:A:290:GLU:OE1	2.44	0.45
1:F:302:MET:HE2	1:F:302:MET:HB3	1.79	0.45
1:F:519:LYS:O	1:F:523:THR:OG1	2.27	0.45
1:I:236:MET:O	1:I:270:ILE:HA	2.15	0.45
1:A:190:PHE:CD1	1:A:204:ILE:HG21	2.51	0.45
1:A:219:THR:HG23	1:A:269:PHE:CE2	2.51	0.45
1:A:447:HIS:CE1	1:A:480:HIS:HB3	2.50	0.45
1:B:327:LEU:O	1:B:333:PHE:HB2	2.17	0.45
1:D:190:PHE:HA	1:D:197:PHE:CE1	2.51	0.45
1:D:577:GLU:O	1:D:581:ILE:HG13	2.17	0.45
1:F:583:LEU:HD13	1:F:583:LEU:HA	1.82	0.45
1:I:519:LYS:O	1:I:523:THR:OG1	2.27	0.45
1:K:599:LYS:O	1:K:601:THR:N	2.46	0.45
1:B:308:HIS:O	1:B:309:THR:HB	2.17	0.45
1:D:251:SER:O	1:D:255:ASP:HB3	2.17	0.45
1:D:516:SER:O	1:D:520:LYS:HG3	2.17	0.45
1:B:295:LEU:HG	1:B:296:ASN:N	2.29	0.45
1:I:298:LEU:O	1:I:302:MET:HG3	2.15	0.45
1:K:344:ILE:HD13	1:K:371:ARG:HB3	1.98	0.45
1:B:213:SER:HB3	1:B:214:PRO:HD2	1.98	0.45
1:B:251:SER:O	1:B:255:ASP:HB3	2.17	0.45
1:F:221:LEU:O	1:F:225:VAL:HG23	2.17	0.45
1:I:447:HIS:CE1	1:I:480:HIS:HB3	2.51	0.45
1:A:171:PHE:H	1:A:228:GLU:CD	2.25	0.45
1:A:494:ALA:C	1:A:496:GLU:N	2.72	0.45
1:B:247:GLY:N	1:B:290:GLU:OE1	2.43	0.45
1:B:278:ARG:HD2	1:B:291:ARG:HD2	1.99	0.45
1:D:221:LEU:O	1:D:225:VAL:HG23	2.17	0.45
1:F:254:ARG:HE	1:F:297:GLN:CD	2.24	0.45
1:F:432:ALA:HB1	1:F:593:ALA:HA	1.97	0.45
1:F:586:LYS:O	1:F:590:VAL:HG23	2.16	0.45
1:I:327:LEU:O	1:I:333:PHE:HB2	2.17	0.45
1:B:221:LEU:O	1:B:225:VAL:HG23	2.17	0.45
1:F:327:LEU:O	1:F:333:PHE:HB2	2.16	0.45
1:I:485:LYS:HA	1:I:488:ILE:HD12	1.98	0.45
1:A:172:LYS:HB2	1:A:172:LYS:HE3	1.70	0.44
1:D:531:VAL:HA	1:D:562:LYS:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLY:O	1:A:496:GLU:HB2	2.18	0.44
1:D:344:ILE:HD13	1:D:371:ARG:HB3	1.98	0.44
1:D:519:LYS:O	1:D:523:THR:OG1	2.26	0.44
1:I:221:LEU:O	1:I:225:VAL:HG23	2.17	0.44
1:I:248:VAL:O	1:I:252:ARG:HG2	2.17	0.44
1:K:577:GLU:O	1:K:581:ILE:HG13	2.16	0.44
1:B:219:THR:HG23	1:B:269:PHE:CE2	2.52	0.44
1:F:191:LEU:HB3	1:F:231:VAL:HG21	2.00	0.44
1:I:219:THR:HG23	1:I:269:PHE:CE2	2.52	0.44
1:F:260:ALA:O	1:F:266:CYS:SG	2.75	0.44
1:F:406:GLU:N	1:F:406:GLU:OE1	2.51	0.44
1:I:498:ILE:HD12	1:I:582:LEU:HB3	1.99	0.44
1:K:327:LEU:O	1:K:333:PHE:HB2	2.17	0.44
1:A:221:LEU:O	1:A:225:VAL:HG23	2.17	0.44
1:A:442:HIS:HB3	1:A:450:PRO:HA	1.99	0.44
1:A:485:LYS:HA	1:A:488:ILE:HD12	2.00	0.44
1:B:490:TYR:O	1:B:491:GLY:C	2.60	0.44
1:D:289:ASP:OD1	1:D:291:ARG:HB3	2.17	0.44
1:I:348:GLU:HA	1:I:351:LEU:HD12	1.99	0.44
1:D:171:PHE:H	1:D:228:GLU:CD	2.26	0.44
1:A:381:LEU:O	1:A:384:LEU:HB3	2.18	0.44
1:D:586:LYS:O	1:D:590:VAL:HG23	2.18	0.44
1:F:171:PHE:H	1:F:228:GLU:CD	2.24	0.44
1:I:302:MET:HE2	1:I:302:MET:HB3	1.83	0.44
1:I:434:HIS:CD2	1:I:438:HIS:HE2	2.34	0.44
1:D:193:ASN:O	1:D:196:LYS:HG2	2.18	0.44
1:D:348:GLU:HA	1:D:351:LEU:HD12	2.00	0.44
1:D:442:HIS:HB3	1:D:450:PRO:HA	1.99	0.44
1:K:171:PHE:H	1:K:228:GLU:CD	2.26	0.44
1:K:221:LEU:O	1:K:225:VAL:HG23	2.17	0.44
1:I:190:PHE:CG	1:I:204:ILE:HG21	2.53	0.43
1:I:483:LEU:O	1:I:487:LYS:HG3	2.17	0.43
1:A:188:VAL:HG12	1:A:192:LYS:HD2	2.00	0.43
1:I:529:GLU:HG2	1:I:569:ARG:NH2	2.33	0.43
1:K:210:LEU:O	1:K:316:ALA:HA	2.19	0.43
1:K:519:LYS:O	1:K:523:THR:OG1	2.29	0.43
1:D:188:VAL:HG12	1:D:192:LYS:HD2	2.00	0.43
1:D:404:ASP:C	1:D:406:GLU:OE1	2.61	0.43
1:I:171:PHE:H	1:I:228:GLU:CD	2.25	0.43
1:B:188:VAL:HG13	1:B:229:ALA:HB2	2.00	0.43
1:F:434:HIS:CD2	1:F:438:HIS:HE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:446:GLU:CG	1:I:447:HIS:CE1	3.02	0.43
1:B:494:ALA:O	1:B:495:SER:C	2.60	0.43
1:B:519:LYS:O	1:B:523:THR:OG1	2.27	0.43
1:D:275:ALA:O	1:D:291:ARG:NH1	2.50	0.43
1:K:254:ARG:HE	1:K:297:GLN:CD	2.26	0.43
1:A:586:LYS:O	1:A:590:VAL:HG23	2.17	0.43
1:D:446:GLU:CG	1:D:447:HIS:CE1	3.02	0.43
1:F:295:LEU:O	1:F:298:LEU:HB3	2.18	0.43
1:F:348:GLU:HA	1:F:351:LEU:HD12	2.00	0.43
1:I:192:LYS:HD2	1:I:229:ALA:HA	2.01	0.43
1:D:178:GLU:OE2	1:D:179:GLU:HG3	2.18	0.43
1:F:219:THR:HG23	1:F:269:PHE:CE2	2.54	0.43
1:F:517:LEU:O	1:F:521:MET:HG3	2.19	0.43
1:F:577:GLU:O	1:F:581:ILE:HG13	2.19	0.43
1:F:592:LEU:HD13	1:F:592:LEU:HA	1.93	0.43
1:I:602:LEU:HD12	1:I:603:THR:H	1.82	0.43
1:K:290:GLU:O	1:K:293:GLN:HG2	2.18	0.43
1:K:446:GLU:CG	1:K:447:HIS:CE1	3.02	0.43
1:K:477:ILE:HB	1:K:482:ILE:HD11	2.01	0.43
1:A:348:GLU:HA	1:A:351:LEU:HD12	2.01	0.43
1:A:446:GLU:CG	1:A:447:HIS:CE1	3.02	0.43
1:I:495:SER:O	1:I:499:ASN:ND2	2.38	0.43
1:K:275:ALA:O	1:K:291:ARG:NH1	2.51	0.43
1:K:516:SER:O	1:K:520:LYS:HG3	2.18	0.43
1:D:327:LEU:O	1:D:333:PHE:HB2	2.17	0.43
1:I:256:LEU:HD21	1:I:268:ILE:HG21	2.00	0.43
1:A:239:SER:HB2	1:B:296:ASN:CG	2.44	0.42
1:F:242:VAL:O	1:F:244:MET:HA	2.19	0.42
1:K:190:PHE:CD1	1:K:204:ILE:HG21	2.54	0.42
1:A:344:ILE:HD13	1:A:371:ARG:HB3	2.02	0.42
1:D:517:LEU:O	1:D:521:MET:HG3	2.19	0.42
1:A:499:ASN:ND2	1:A:589:LEU:HD21	2.30	0.42
1:D:191:LEU:HB3	1:D:231:VAL:HG21	2.01	0.42
1:F:446:GLU:CG	1:F:447:HIS:CE1	3.02	0.42
1:B:494:ALA:C	1:B:496:GLU:N	2.74	0.42
1:D:190:PHE:CD1	1:D:204:ILE:HG21	2.55	0.42
1:A:479:LYS:HG3	1:A:521:MET:HE3	2.01	0.42
1:B:297:GLN:O	1:B:298:LEU:C	2.63	0.42
1:B:516:SER:O	1:B:520:LYS:HG3	2.18	0.42
1:F:188:VAL:HG13	1:F:229:ALA:HB2	2.01	0.42
1:K:348:GLU:HA	1:K:351:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:O	1:A:316:ALA:HA	2.19	0.42
1:D:236:MET:HB3	1:D:241:PHE:CZ	2.55	0.42
1:K:260:ALA:O	1:K:266:CYS:SG	2.74	0.42
1:A:365:ASN:ND2	1:A:368:VAL:H	2.16	0.42
1:A:517:LEU:O	1:A:521:MET:HG3	2.19	0.42
1:I:236:MET:HB3	1:I:241:PHE:CZ	2.55	0.42
1:K:354:HIS:HB2	1:K:385:ILE:HD12	2.00	0.42
1:A:317:THR:HG21	1:A:323:LEU:HD11	2.01	0.42
1:D:188:VAL:HG13	1:D:229:ALA:HB2	2.01	0.42
1:K:191:LEU:HB3	1:K:231:VAL:HG21	2.01	0.42
1:B:210:LEU:O	1:B:316:ALA:HA	2.20	0.42
1:F:210:LEU:O	1:F:316:ALA:HA	2.20	0.42
1:F:498:ILE:HD12	1:F:582:LEU:HB3	2.02	0.42
1:B:303:ASP:O	1:B:305:PHE:N	2.53	0.41
1:B:577:GLU:O	1:B:581:ILE:HG13	2.20	0.41
1:I:602:LEU:HG	1:I:603:THR:N	2.35	0.41
1:A:241:PHE:CZ	1:A:256:LEU:HD22	2.44	0.41
1:A:529:GLU:H	1:A:529:GLU:HG2	1.70	0.41
1:B:236:MET:HB3	1:B:241:PHE:CZ	2.55	0.41
1:B:454:VAL:O	1:B:601:THR:HA	2.20	0.41
1:I:574:CYS:O	1:I:575:LEU:C	2.61	0.41
1:K:478:ASN:HB2	1:K:481:GLN:HG3	2.03	0.41
1:B:183:GLU:O	1:B:186:GLU:HG2	2.20	0.41
1:B:494:ALA:O	1:B:496:GLU:N	2.53	0.41
1:K:171:PHE:HD1	1:K:224:ALA:HB1	1.84	0.41
1:A:297:GLN:O	1:A:300:VAL:HB	2.20	0.41
1:F:190:PHE:CD1	1:F:204:ILE:HG21	2.56	0.41
1:F:317:THR:HG21	1:F:323:LEU:HD11	2.03	0.41
1:B:348:GLU:HA	1:B:351:LEU:HD12	2.01	0.41
1:D:302:MET:HE2	1:D:302:MET:HB3	1.83	0.41
1:I:210:LEU:O	1:I:316:ALA:HA	2.20	0.41
1:I:517:LEU:O	1:I:521:MET:HG3	2.20	0.41
1:K:517:LEU:O	1:K:521:MET:HG3	2.20	0.41
1:B:211:VAL:HG13	1:B:317:THR:HG23	2.03	0.41
1:A:275:ALA:O	1:A:291:ARG:NH1	2.54	0.41
1:A:296:ASN:O	1:A:300:VAL:HG23	2.21	0.41
1:A:457:ILE:HD13	1:A:457:ILE:O	2.21	0.41
1:A:598:LEU:HG	1:A:599:LYS:N	2.35	0.41
1:F:236:MET:HB3	1:F:241:PHE:CZ	2.56	0.41
1:F:596:LEU:HD13	1:F:596:LEU:HA	1.89	0.41
1:F:213:SER:HB3	1:F:214:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:ALA:O	1:F:291:ARG:NH1	2.51	0.41
1:I:518:ALA:O	1:I:522:VAL:HG23	2.20	0.41
1:K:596:LEU:O	1:K:600:GLU:N	2.49	0.41
1:A:577:GLU:O	1:A:581:ILE:HG13	2.21	0.41
1:B:517:LEU:O	1:B:521:MET:HG3	2.19	0.41
1:D:204:ILE:HG23	1:D:205:PRO:HD2	2.02	0.41
1:F:529:GLU:H	1:F:529:GLU:HG2	1.69	0.41
1:I:558:ASN:O	1:I:562:LYS:HG3	2.21	0.41
1:A:519:LYS:O	1:A:523:THR:OG1	2.27	0.41
1:B:260:ALA:O	1:B:266:CYS:SG	2.74	0.41
1:B:482:ILE:O	1:B:486:ILE:HG13	2.21	0.41
1:D:210:LEU:O	1:D:316:ALA:HA	2.20	0.41
1:F:478:ASN:HB2	1:F:481:GLN:HG3	2.03	0.41
1:I:266:CYS:SG	1:I:311:VAL:HG12	2.62	0.41
1:K:317:THR:HG21	1:K:323:LEU:HD11	2.02	0.41
1:B:269:PHE:HA	1:B:314:MET:O	2.22	0.40
1:I:569:ARG:O	1:I:573:GLU:HG3	2.21	0.40
1:K:596:LEU:HD12	1:K:596:LEU:HA	1.71	0.40
1:A:495:SER:HB3	1:A:589:LEU:HD11	2.03	0.40
1:A:568:LYS:O	1:A:572:GLU:HG3	2.22	0.40
1:D:498:ILE:HD12	1:D:582:LEU:HB3	2.03	0.40
1:F:269:PHE:HA	1:F:314:MET:O	2.21	0.40
1:F:497:GLN:O	1:F:501:GLY:HA2	2.21	0.40
1:I:269:PHE:HA	1:I:314:MET:O	2.21	0.40
1:D:478:ASN:HB2	1:D:481:GLN:HG3	2.04	0.40
1:F:477:ILE:HB	1:F:482:ILE:HD11	2.03	0.40
1:I:260:ALA:O	1:I:266:CYS:SG	2.74	0.40
1:K:250:ALA:O	1:K:253:VAL:HB	2.21	0.40
1:K:258:ASP:O	1:K:261:ARG:CG	2.69	0.40
1:K:323:LEU:HB3	1:K:327:LEU:HD12	2.03	0.40
1:D:406:GLU:OE1	1:D:407:GLU:HG2	2.21	0.40
1:I:171:PHE:HD1	1:I:224:ALA:HB1	1.87	0.40
1:I:563:VAL:O	1:I:567:VAL:HG23	2.20	0.40
1:A:563:VAL:O	1:A:567:VAL:HG23	2.22	0.40
1:B:192:LYS:NZ	1:B:228:GLU:O	2.52	0.40
1:F:434:HIS:HE1	1:F:510:ASP:OD1	2.05	0.40
1:F:588:GLN:O	1:F:591:LYS:HB2	2.22	0.40
1:K:175:ALA:HB2	1:K:353:ILE:HD11	2.04	0.40
1:K:393:ALA:HB3	1:K:394:ARG:HH12	1.85	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	352/453 (78%)	325 (92%)	23 (6%)	4 (1%)	11	39
1	B	360/453 (80%)	331 (92%)	23 (6%)	6 (2%)	7	30
1	D	350/453 (77%)	325 (93%)	23 (7%)	2 (1%)	21	52
1	F	351/453 (78%)	327 (93%)	21 (6%)	3 (1%)	14	43
1	I	351/453 (78%)	326 (93%)	22 (6%)	3 (1%)	14	43
1	K	352/453 (78%)	325 (92%)	23 (6%)	4 (1%)	11	39
All	All	2116/2718 (78%)	1959 (93%)	135 (6%)	22 (1%)	12	40

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	245	PHE
1	B	245	PHE
1	B	304	GLY
1	D	245	PHE
1	F	178	GLU
1	F	245	PHE
1	I	178	GLU
1	I	245	PHE
1	K	178	GLU
1	K	245	PHE
1	A	494	ALA
1	B	303	ASP
1	B	305	PHE
1	A	495	SER
1	I	333	PHE
1	K	289	ASP
1	B	178	GLU
1	B	333	PHE
1	D	333	PHE

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Mol	Chain	Res	Type
1	F	333	PHE
1	K	333	PHE

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	259/375 (69%)	193 (74%)	66 (26%)	0	3
1	B	263/375 (70%)	199 (76%)	64 (24%)	1	3
1	D	256/375 (68%)	197 (77%)	59 (23%)	1	4
1	F	257/375 (68%)	194 (76%)	63 (24%)	1	3
1	I	260/375 (69%)	194 (75%)	66 (25%)	0	3
1	K	259/375 (69%)	197 (76%)	62 (24%)	1	4
All	All	1554/2250 (69%)	1174 (76%)	380 (24%)	1	3

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	A	174	VAL
1	A	178	GLU
1	A	179	GLU
1	A	185	ARG
1	A	196	LYS
1	A	200	ILE
1	A	206	LYS
1	A	211	VAL
1	A	213	SER
1	A	220	LEU
1	A	231	VAL
1	A	232	SER
1	A	237	SER
1	A	251	SER
1	A	252	ARG

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Mol	Chain	Res	Type
1	A	254	ARG
1	A	256	LEU
1	A	272	GLU
1	A	274	ASP
1	A	276	VAL
1	A	288	HIS
1	A	290	GLU
1	A	291	ARG
1	A	295	LEU
1	A	298	LEU
1	A	302	MET
1	A	303	ASP
1	A	305	PHE
1	A	312	ILE
1	A	321	ASP
1	A	328	LEU
1	A	329	ARG
1	A	332	ARG
1	A	335	ARG
1	A	340	SER
1	A	344	ILE
1	A	358	THR
1	A	360	LEU
1	A	369	ILE
1	A	371	ARG
1	A	377	SER
1	A	386	ASN
1	A	406	GLU
1	A	424	THR
1	A	431	THR
1	A	454	VAL
1	A	455	THR
1	A	457	ILE
1	A	459	ARG
1	A	477	ILE
1	A	495	SER
1	A	497	GLN
1	A	520	LYS
1	A	529	GLU
1	A	537	VAL
1	A	579	SER
1	A	583	LEU

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Mol	Chain	Res	Type
1	A	587	ASP
1	A	589	LEU
1	A	592	LEU
1	A	594	LYS
1	A	596	LEU
1	A	598	LEU
1	A	599	LYS
1	A	603	THR
1	B	172	LYS
1	B	174	VAL
1	B	179	GLU
1	B	185	ARG
1	B	196	LYS
1	B	200	ILE
1	B	206	LYS
1	B	211	VAL
1	B	213	SER
1	B	231	VAL
1	B	232	SER
1	B	237	SER
1	B	241	PHE
1	B	242	VAL
1	B	251	SER
1	B	252	ARG
1	B	255	ASP
1	B	256	LEU
1	B	274	ASP
1	B	276	VAL
1	B	278	ARG
1	B	290	GLU
1	B	293	GLN
1	B	295	LEU
1	B	298	LEU
1	B	300	VAL
1	B	302	MET
1	B	307	THR
1	B	312	ILE
1	B	321	ASP
1	B	328	LEU
1	B	332	ARG
1	B	335	ARG
1	B	344	ILE

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Mol	Chain	Res	Type
1	B	360	LEU
1	B	369	ILE
1	B	371	ARG
1	B	386	ASN
1	B	394	ARG
1	B	403	LYS
1	B	404	ASP
1	B	407	GLU
1	B	431	THR
1	B	446	GLU
1	B	452	HIS
1	B	477	ILE
1	B	495	SER
1	B	497	GLN
1	B	509	ASN
1	B	529	GLU
1	B	537	VAL
1	B	558	ASN
1	B	562	LYS
1	B	566	GLU
1	B	579	SER
1	B	583	LEU
1	B	587	ASP
1	B	589	LEU
1	B	592	LEU
1	B	594	LYS
1	B	596	LEU
1	B	599	LYS
1	B	602	LEU
1	B	603	THR
1	D	174	VAL
1	D	178	GLU
1	D	179	GLU
1	D	185	ARG
1	D	196	LYS
1	D	200	ILE
1	D	206	LYS
1	D	211	VAL
1	D	213	SER
1	D	220	LEU
1	D	231	VAL
1	D	232	SER

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Mol	Chain	Res	Type
1	D	237	SER
1	D	241	PHE
1	D	251	SER
1	D	252	ARG
1	D	255	ASP
1	D	256	LEU
1	D	274	ASP
1	D	293	GLN
1	D	298	LEU
1	D	312	ILE
1	D	321	ASP
1	D	328	LEU
1	D	329	ARG
1	D	332	ARG
1	D	335	ARG
1	D	344	ILE
1	D	360	LEU
1	D	369	ILE
1	D	371	ARG
1	D	377	SER
1	D	386	ASN
1	D	394	ARG
1	D	403	LYS
1	D	406	GLU
1	D	407	GLU
1	D	424	THR
1	D	431	THR
1	D	452	HIS
1	D	454	VAL
1	D	477	ILE
1	D	495	SER
1	D	497	GLN
1	D	509	ASN
1	D	529	GLU
1	D	537	VAL
1	D	558	ASN
1	D	566	GLU
1	D	583	LEU
1	D	584	LYS
1	D	587	ASP
1	D	589	LEU
1	D	592	LEU

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Mol	Chain	Res	Type
1	D	594	LYS
1	D	596	LEU
1	D	598	LEU
1	D	599	LYS
1	D	602	LEU
1	F	174	VAL
1	F	178	GLU
1	F	179	GLU
1	F	185	ARG
1	F	192	LYS
1	F	196	LYS
1	F	200	ILE
1	F	206	LYS
1	F	211	VAL
1	F	213	SER
1	F	220	LEU
1	F	231	VAL
1	F	232	SER
1	F	237	SER
1	F	241	PHE
1	F	242	VAL
1	F	248	VAL
1	F	251	SER
1	F	252	ARG
1	F	254	ARG
1	F	256	LEU
1	F	272	GLU
1	F	274	ASP
1	F	278	ARG
1	F	290	GLU
1	F	291	ARG
1	F	293	GLN
1	F	295	LEU
1	F	312	ILE
1	F	321	ASP
1	F	328	LEU
1	F	332	ARG
1	F	335	ARG
1	F	344	ILE
1	F	360	LEU
1	F	369	ILE
1	F	371	ARG

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Mol	Chain	Res	Type
1	F	377	SER
1	F	386	ASN
1	F	394	ARG
1	F	403	LYS
1	F	404	ASP
1	F	406	GLU
1	F	407	GLU
1	F	410	ASP
1	F	424	THR
1	F	431	THR
1	F	477	ILE
1	F	497	GLN
1	F	509	ASN
1	F	529	GLU
1	F	537	VAL
1	F	558	ASN
1	F	566	GLU
1	F	579	SER
1	F	583	LEU
1	F	587	ASP
1	F	589	LEU
1	F	592	LEU
1	F	594	LYS
1	F	596	LEU
1	F	598	LEU
1	F	602	LEU
1	I	172	LYS
1	I	174	VAL
1	I	178	GLU
1	I	179	GLU
1	I	185	ARG
1	I	192	LYS
1	I	200	ILE
1	I	204	ILE
1	I	206	LYS
1	I	211	VAL
1	I	220	LEU
1	I	228	GLU
1	I	231	VAL
1	I	232	SER
1	I	237	SER
1	I	239	SER

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Mol	Chain	Res	Type
1	I	241	PHE
1	I	242	VAL
1	I	246	VAL
1	I	251	SER
1	I	252	ARG
1	I	254	ARG
1	I	259	ASN
1	I	274	ASP
1	I	276	VAL
1	I	278	ARG
1	I	290	GLU
1	I	293	GLN
1	I	295	LEU
1	I	298	LEU
1	I	312	ILE
1	I	321	ASP
1	I	328	LEU
1	I	329	ARG
1	I	332	ARG
1	I	335	ARG
1	I	340	SER
1	I	344	ILE
1	I	358	THR
1	I	360	LEU
1	I	369	ILE
1	I	371	ARG
1	I	377	SER
1	I	385	ILE
1	I	394	ARG
1	I	403	LYS
1	I	404	ASP
1	I	424	THR
1	I	431	THR
1	I	454	VAL
1	I	457	ILE
1	I	477	ILE
1	I	486	ILE
1	I	495	SER
1	I	497	GLN
1	I	509	ASN
1	I	520	LYS
1	I	529	GLU

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Mol	Chain	Res	Type
1	I	537	VAL
1	I	579	SER
1	I	583	LEU
1	I	587	ASP
1	I	592	LEU
1	I	594	LYS
1	I	596	LEU
1	I	598	LEU
1	K	172	LYS
1	K	174	VAL
1	K	179	GLU
1	K	185	ARG
1	K	200	ILE
1	K	206	LYS
1	K	211	VAL
1	K	213	SER
1	K	220	LEU
1	K	228	GLU
1	K	231	VAL
1	K	232	SER
1	K	237	SER
1	K	241	PHE
1	K	242	VAL
1	K	251	SER
1	K	252	ARG
1	K	254	ARG
1	K	256	LEU
1	K	274	ASP
1	K	276	VAL
1	K	278	ARG
1	K	289	ASP
1	K	293	GLN
1	K	295	LEU
1	K	298	LEU
1	K	312	ILE
1	K	321	ASP
1	K	328	LEU
1	K	332	ARG
1	K	335	ARG
1	K	340	SER
1	K	344	ILE
1	K	360	LEU

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Mol	Chain	Res	Type
1	K	369	ILE
1	K	371	ARG
1	K	377	SER
1	K	385	ILE
1	K	394	ARG
1	K	403	LYS
1	K	424	THR
1	K	431	THR
1	K	454	VAL
1	K	477	ILE
1	K	486	ILE
1	K	495	SER
1	K	509	ASN
1	K	513	GLN
1	K	529	GLU
1	K	537	VAL
1	K	566	GLU
1	K	579	SER
1	K	583	LEU
1	K	584	LYS
1	K	587	ASP
1	K	589	LEU
1	K	592	LEU
1	K	594	LYS
1	K	596	LEU
1	K	598	LEU
1	K	599	LYS
1	K	603	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	ASN
1	A	447	HIS
1	A	478	ASN
1	A	499	ASN
1	B	296	ASN
1	B	297	GLN
1	B	383	ASN
1	B	447	HIS
1	B	478	ASN
1	D	297	GLN

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Mol	Chain	Res	Type
1	D	318	ASN
1	D	447	HIS
1	D	478	ASN
1	D	499	ASN
1	D	558	ASN
1	F	297	GLN
1	F	447	HIS
1	F	478	ASN
1	F	499	ASN
1	I	296	ASN
1	I	297	GLN
1	I	383	ASN
1	I	447	HIS
1	I	478	ASN
1	K	293	GLN
1	K	297	GLN
1	K	447	HIS
1	K	478	ASN
1	K	558	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	701	-	28,29,29	0.52	0	43,45,45	0.63	0
2	ADP	I	701	-	28,29,29	0.64	0	43,45,45	0.66	1 (2%)
2	ADP	B	701	-	28,29,29	0.57	0	43,45,45	0.58	0
2	ADP	D	701	-	28,29,29	0.57	0	43,45,45	0.62	0
2	ADP	F	701	-	28,29,29	1.01	1 (3%)	43,45,45	1.23	4 (9%)
2	ADP	K	701	-	28,29,29	0.67	0	43,45,45	0.70	1 (2%)

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	ADP	A	701	-	-	2/16/32/32	0/3/3/3
2	ADP	I	701	-	-	0/16/32/32	0/3/3/3
2	ADP	B	701	-	-	2/16/32/32	0/3/3/3
2	ADP	D	701	-	-	2/16/32/32	0/3/3/3
2	ADP	F	701	-	-	1/16/32/32	0/3/3/3
2	ADP	K	701	-	-	1/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	ADP	C5-N7	2.39	1.43	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	701	ADP	C5-C4-N9	4.07	110.24	105.81
2	F	701	ADP	C6-C5-C4	3.24	121.60	117.18
2	F	701	ADP	C4-C5-N7	-2.59	107.62	110.58
2	K	701	ADP	O2A-PA-O3A	2.22	113.27	107.27
2	F	701	ADP	O2A-PA-O3A	2.17	113.14	107.27
2	I	701	ADP	O2A-PA-O3A	2.10	112.96	107.27

There are no chirality outliers.

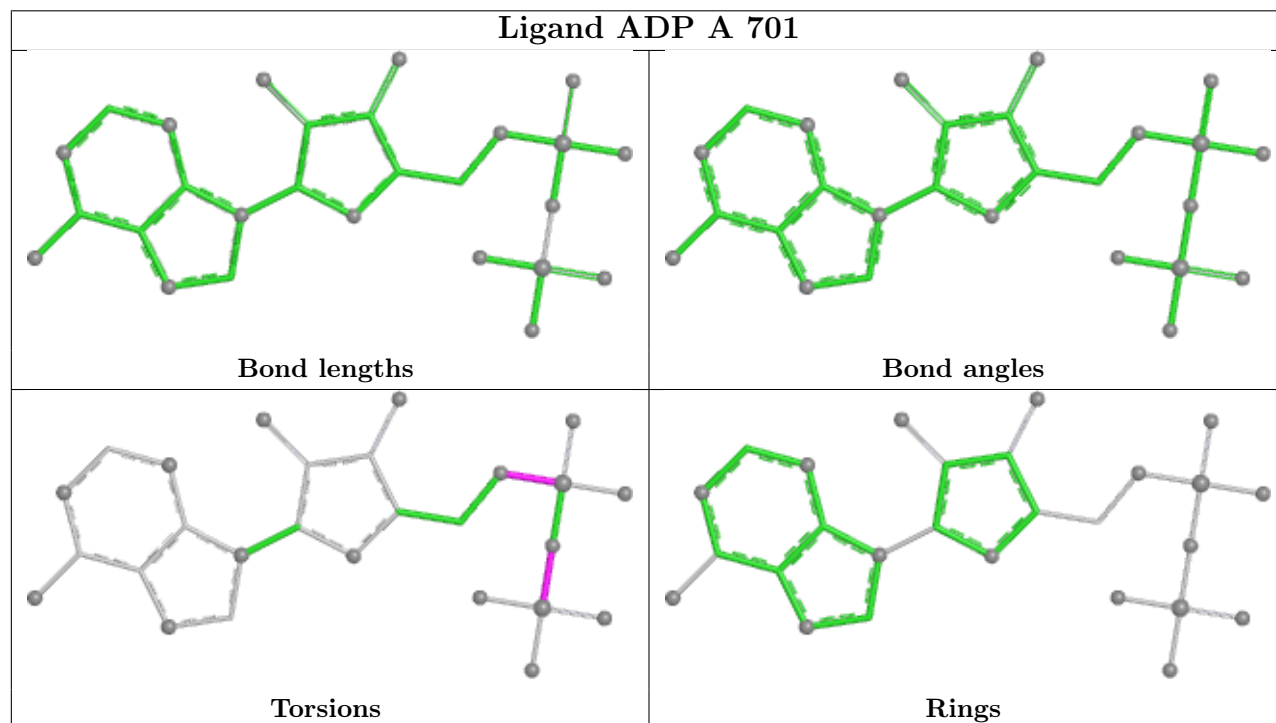
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ADP	C5'-O5'-PA-O1A
2	B	701	ADP	C5'-O5'-PA-O1A
2	D	701	ADP	C5'-O5'-PA-O1A
2	A	701	ADP	PA-O3A-PB-O2B
2	B	701	ADP	PA-O3A-PB-O2B
2	D	701	ADP	PA-O3A-PB-O2B
2	F	701	ADP	PA-O3A-PB-O2B
2	K	701	ADP	PA-O3A-PB-O2B

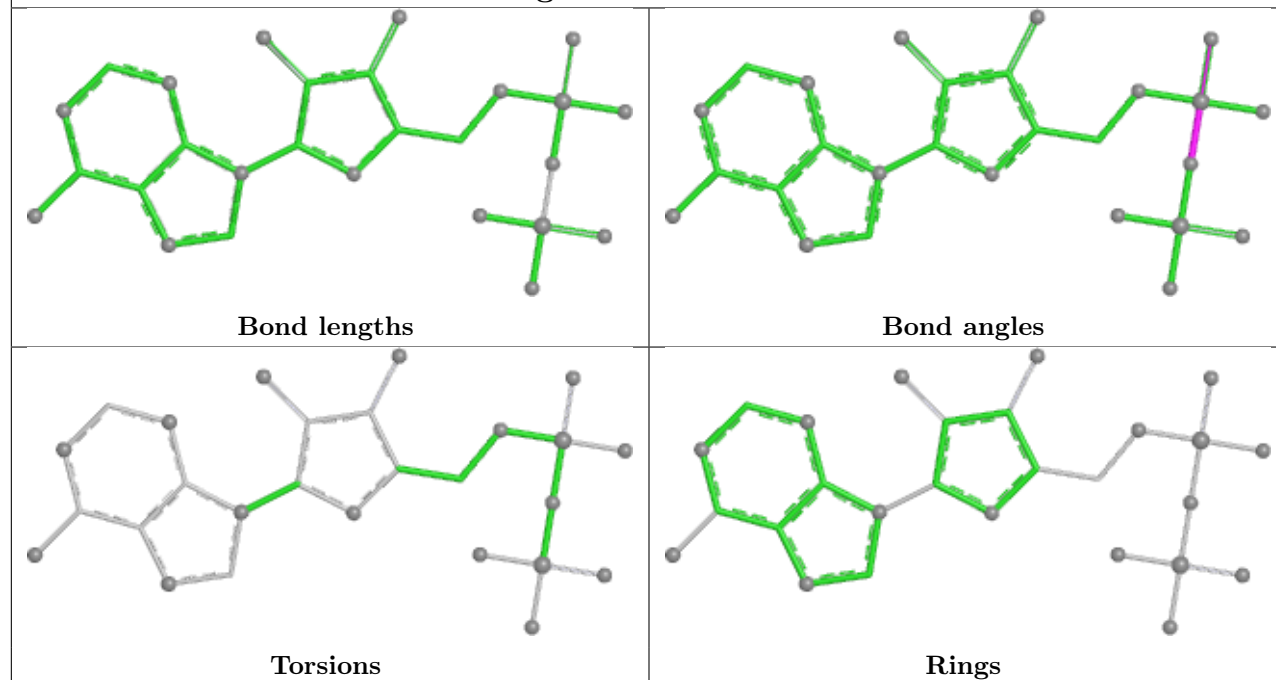
There are no ring outliers.

No monomer is involved in short contacts.

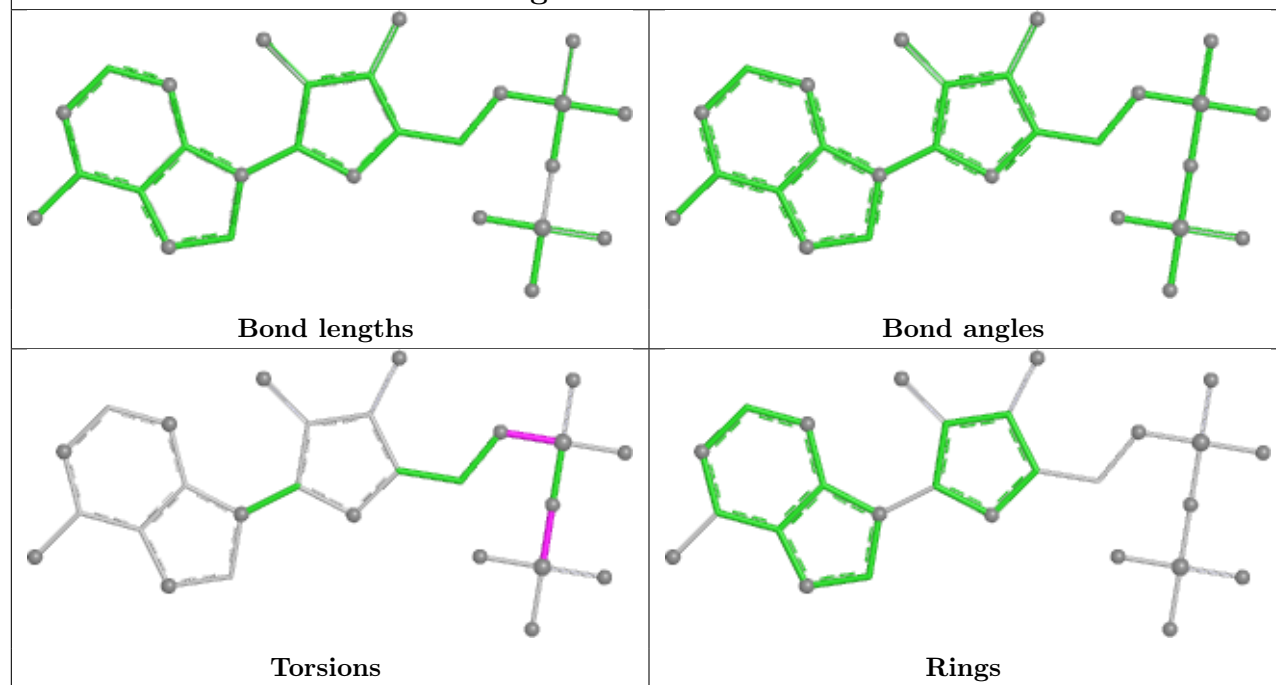
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

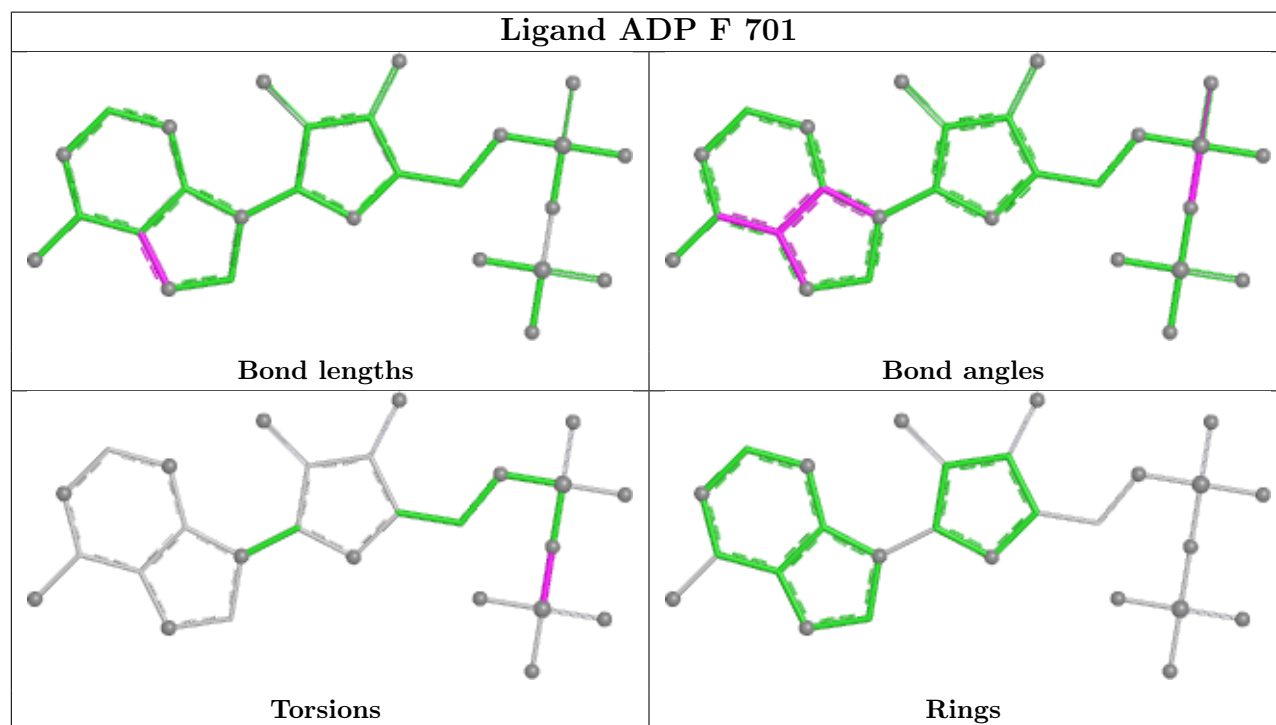
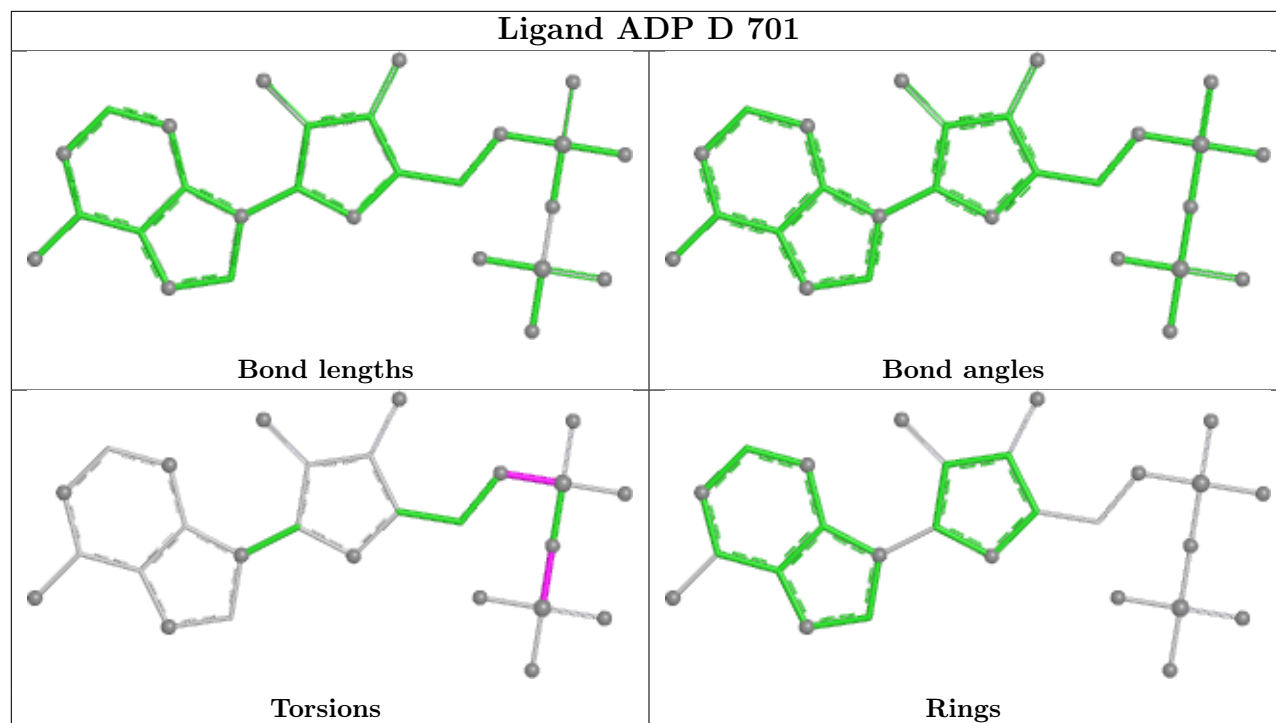


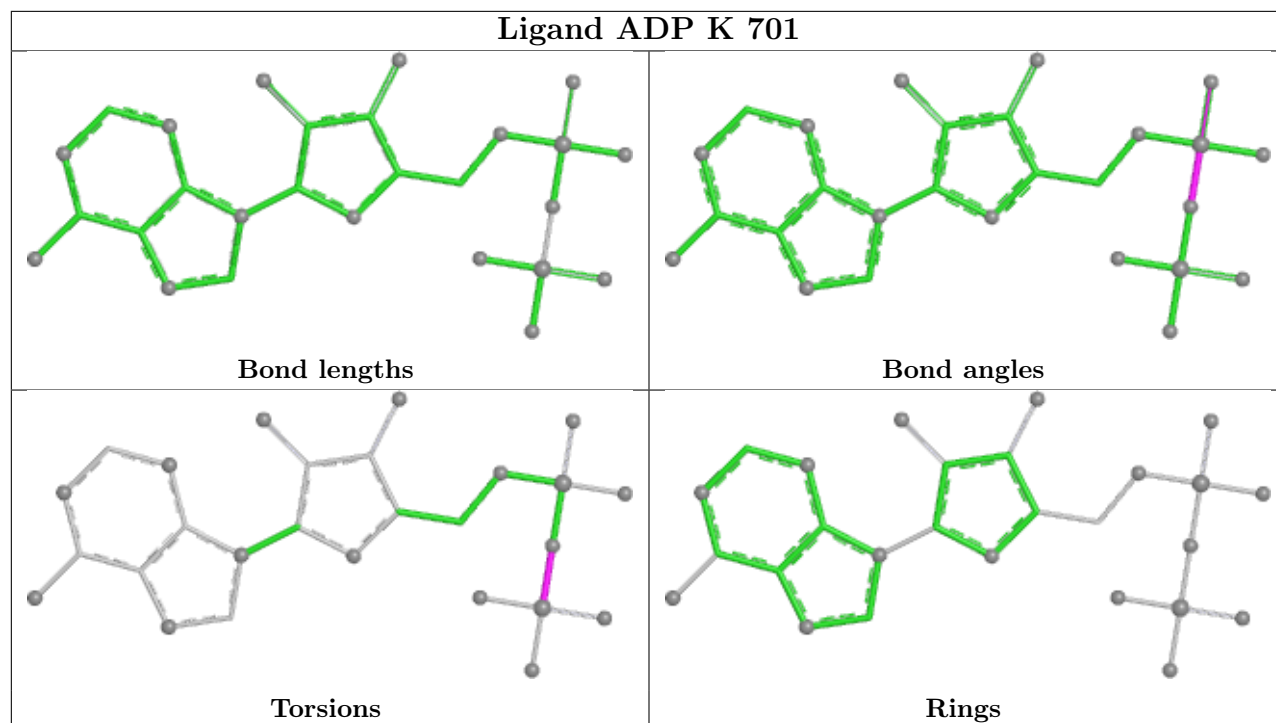
Ligand ADP I 701



Ligand ADP B 701







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	368/453 (81%)	0.20	5 (1%) 73 55	63, 122, 174, 225	0
1	B	374/453 (82%)	0.44	14 (3%) 45 31	60, 131, 191, 246	0
1	D	366/453 (80%)	0.19	7 (1%) 66 48	68, 128, 184, 256	0
1	F	367/453 (81%)	0.27	7 (1%) 66 48	63, 136, 201, 233	0
1	I	367/453 (81%)	0.26	14 (3%) 44 30	68, 133, 192, 254	0
1	K	368/453 (81%)	0.24	9 (2%) 59 40	68, 134, 189, 257	0
All	All	2210/2718 (81%)	0.27	56 (2%) 58 39	60, 131, 190, 257	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	577	GLU	4.0
1	A	217	GLY	3.7
1	I	560	ALA	3.3
1	K	211	VAL	3.2
1	I	524	GLU	3.2
1	F	247	GLY	3.2
1	B	328	LEU	3.0
1	D	217	GLY	2.9
1	B	317	THR	2.9
1	D	486	ILE	2.8
1	B	316	ALA	2.8
1	B	320	PRO	2.8
1	F	457	ILE	2.8
1	A	460	GLY	2.7
1	A	525	TRP	2.7
1	F	603	THR	2.7
1	F	190	PHE	2.7
1	B	255	ASP	2.7
1	I	525	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	560	ALA	2.6
1	I	603	THR	2.6
1	B	217	GLY	2.6
1	K	603	THR	2.6
1	K	457	ILE	2.5
1	K	577	GLU	2.4
1	D	234	PHE	2.4
1	B	190	PHE	2.4
1	D	602	LEU	2.4
1	I	369	ILE	2.3
1	I	442	HIS	2.3
1	I	596	LEU	2.3
1	A	577	GLU	2.3
1	B	476	SER	2.3
1	I	187	VAL	2.3
1	B	348	GLU	2.2
1	B	315	ALA	2.2
1	I	579	SER	2.2
1	F	217	GLY	2.2
1	D	562	LYS	2.2
1	K	530	GLU	2.2
1	B	302	MET	2.1
1	I	412	ILE	2.1
1	I	217	GLY	2.1
1	A	434	HIS	2.1
1	D	534	ILE	2.1
1	I	378	GLY	2.1
1	B	323	LEU	2.1
1	D	434	HIS	2.1
1	K	592	LEU	2.1
1	K	395	ASN	2.1
1	I	259	ASN	2.0
1	B	434	HIS	2.0
1	F	375	GLY	2.0
1	K	277	GLY	2.0
1	I	342	PRO	2.0
1	K	257	PHE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

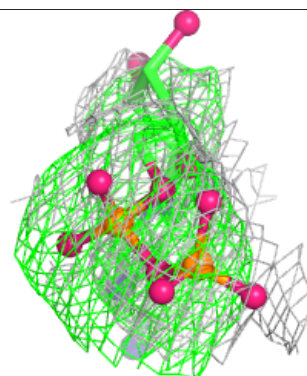
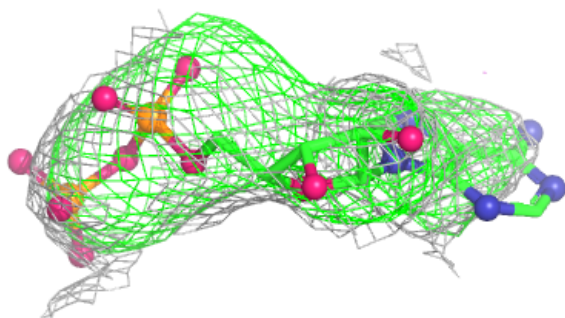
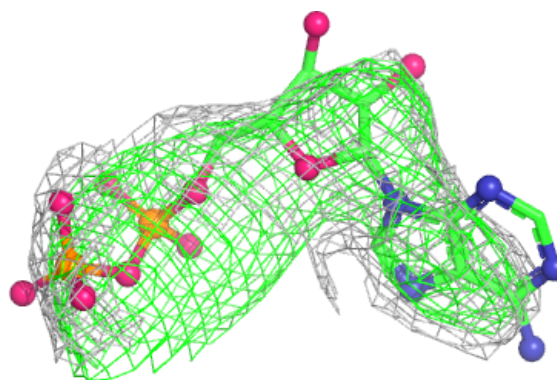
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	A	701	27/27	-	-	84,120,149,157	27
2	ADP	B	701	27/27	-	-	95,131,160,167	27
2	ADP	D	701	27/27	-	-	97,133,161,169	27
2	ADP	F	701	27/27	-	-	97,133,161,169	27
2	ADP	I	701	27/27	-	-	98,134,163,171	27
2	ADP	K	701	27/27	-	-	100,136,165,172	27
3	ZN	A	702	1/1	-	-	66,66,66,66	1
3	ZN	B	702	1/1	-	-	77,77,77,77	1
3	ZN	D	702	1/1	-	-	79,79,79,79	1
3	ZN	F	702	1/1	-	-	79,79,79,79	1
3	ZN	I	702	1/1	-	-	80,80,80,80	1
3	ZN	K	702	1/1	-	-	82,82,82,82	1

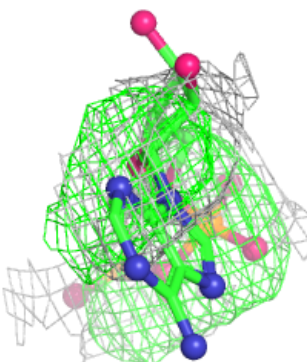
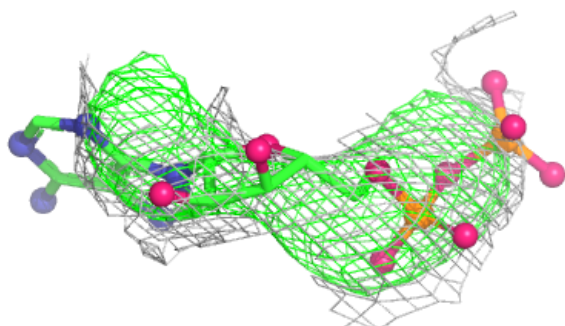
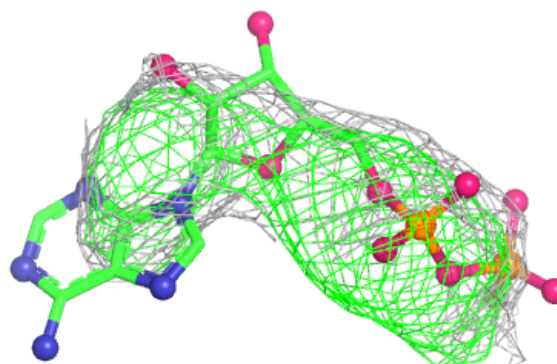
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 701:

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

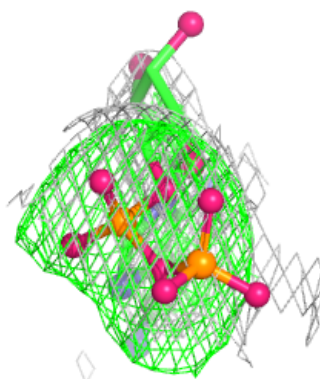
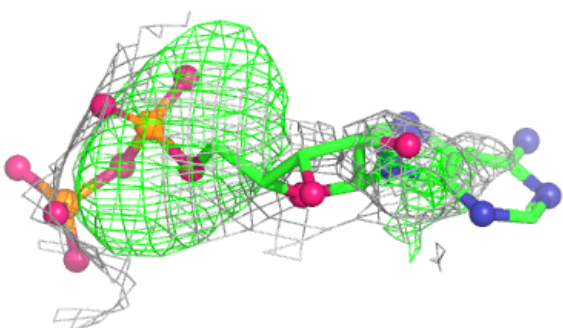
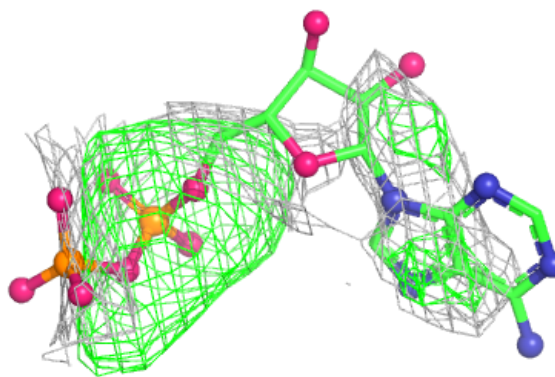
**Electron density around ADP B 701:**

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

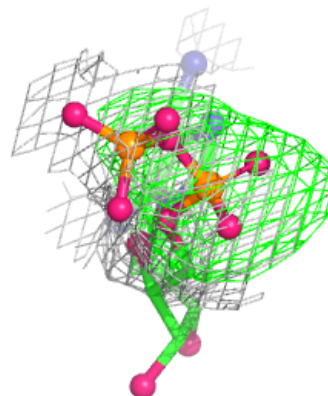
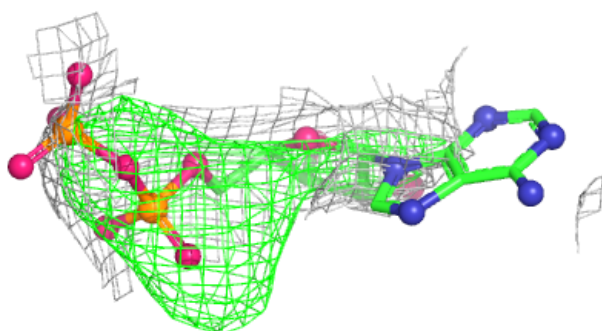
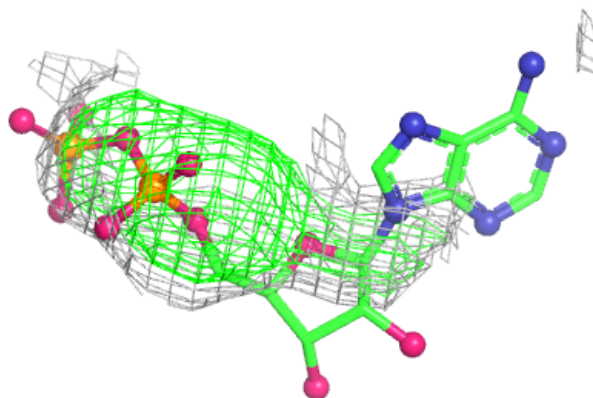


Electron density around ADP D 701:

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

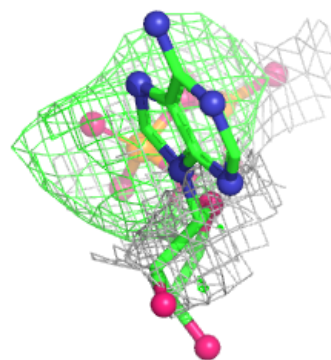
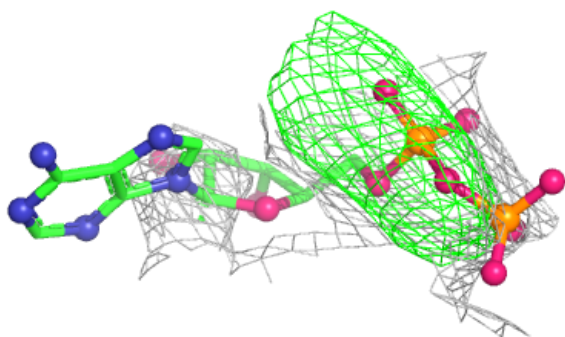
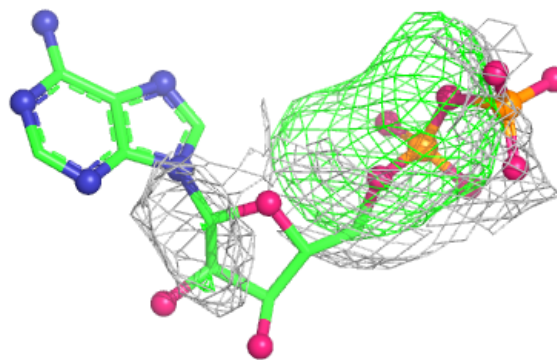
**Electron density around ADP F 701:**

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

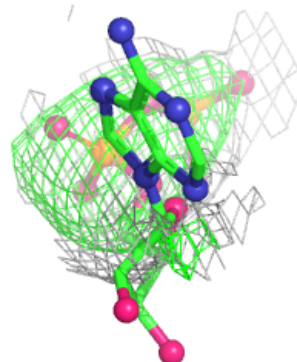
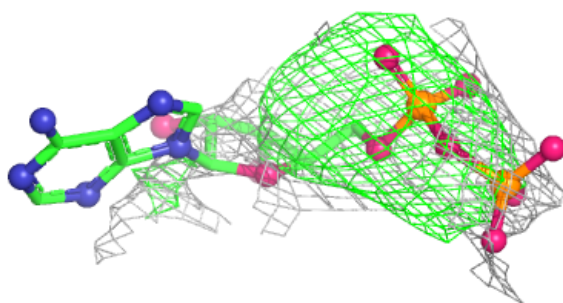
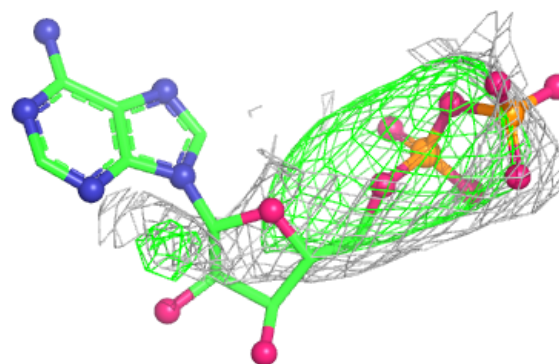


Electron density around ADP I 701:

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

**Electron density around ADP K 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.