



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 12:08 PM UTC

PDB ID : 1XDP / pdb_00001xdp
Title : Crystal Structure of the E.coli Polyphosphate Kinase in complex with AMPPNP
Authors : Zhu, Y.; Huang, W.; Lee, S.S.; Xu, W.
Deposited on : 2004-09-07
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

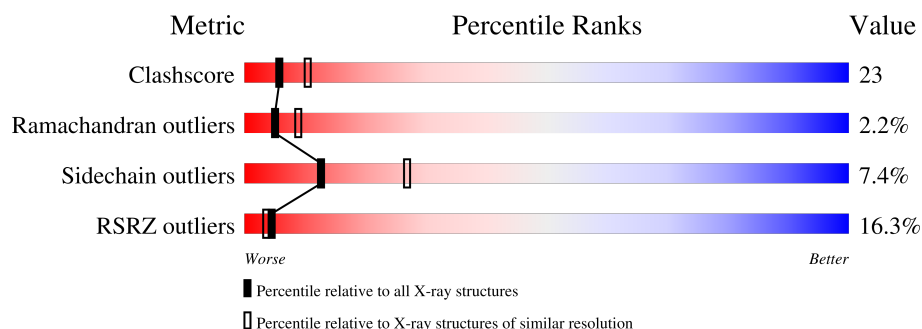
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	687	
1	B	687	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	703	-	-	-	X
2	MG	B	705	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	B	706	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11538 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.

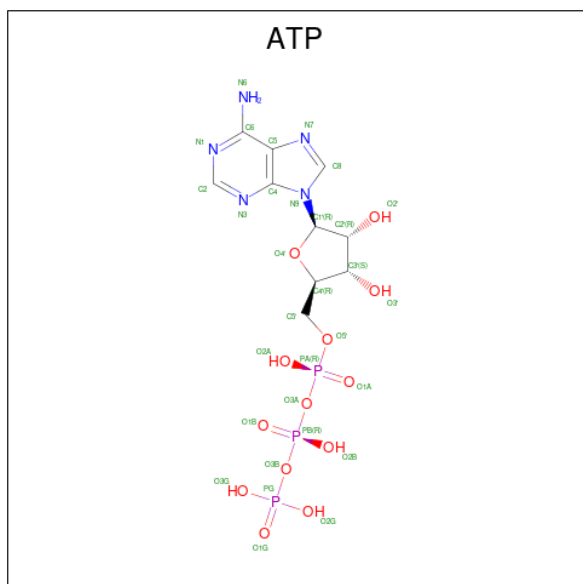
- Molecule 1 is a protein called Polyphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5671	3621	1008	1026	16			
1	B	687	Total	C	N	O	S	0	0	0
			5671	3621	1008	1026	16			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

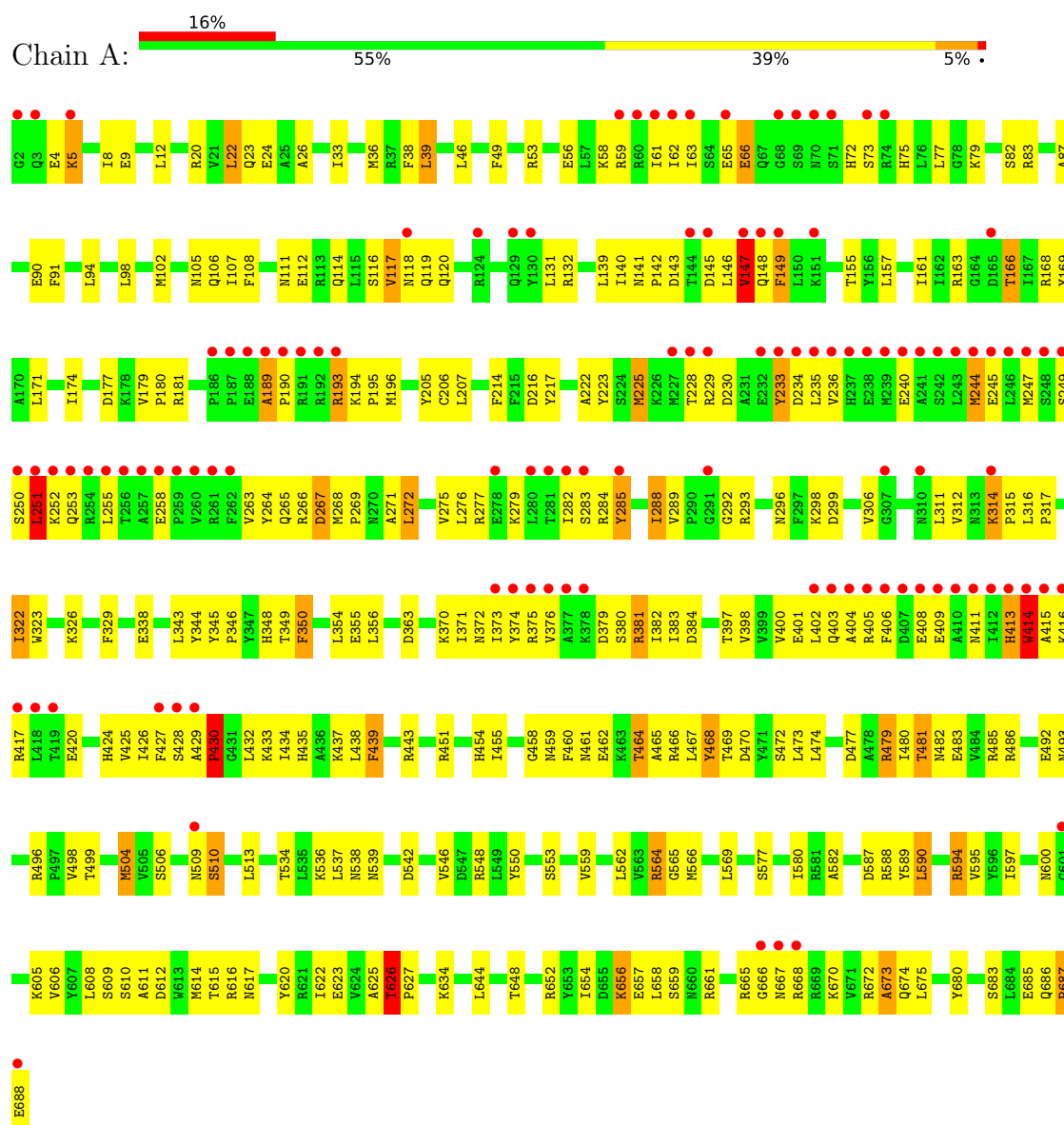
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	54	Total	O	0	0
			54	54		

3 Residue-property plots [i](#)

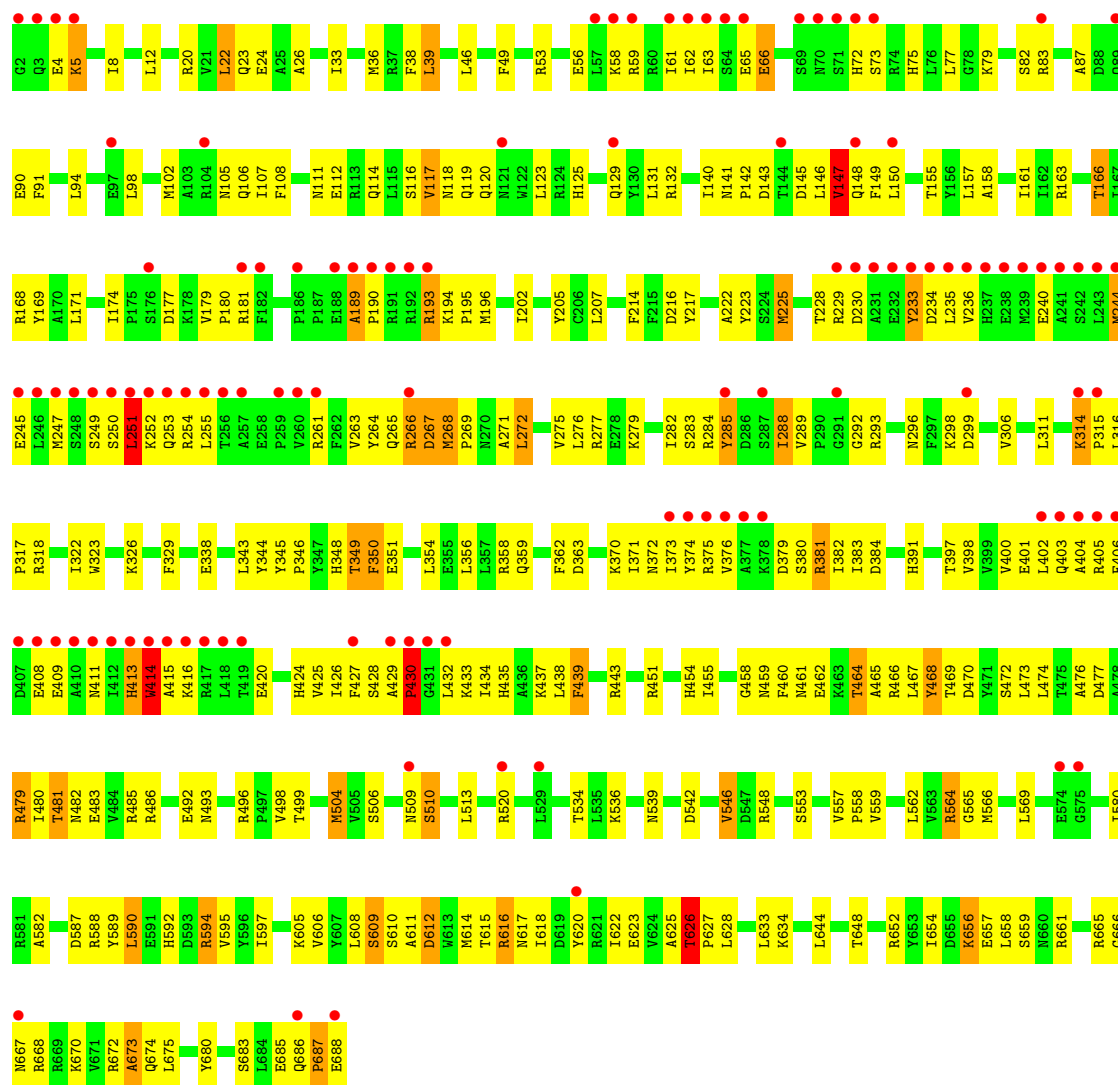
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Polyphosphate kinase



• Molecule 1: Polyphosphate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.00Å 152.00Å 150.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 98.2 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.274 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -h,-l,-k 0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11538	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/5789	1.04	33/7825 (0.4%)
1	B	0.50	1/5789 (0.0%)	1.03	36/7825 (0.5%)
All	All	0.50	1/11578 (0.0%)	1.03	69/15650 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	MET	SD-CE	-5.42	1.66	1.79

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	ARG	NE-CZ-NH2	12.41	130.37	119.20
1	A	594	ARG	CD-NE-CZ	10.53	139.14	124.40
1	B	594	ARG	NE-CZ-NH1	8.69	130.19	121.50
1	B	594	ARG	CD-NE-CZ	8.56	136.38	124.40
1	B	350	PHE	N-CA-C	-8.07	103.43	113.28
1	B	381	ARG	N-CA-C	-7.97	102.82	112.54
1	A	381	ARG	N-CA-C	-7.81	102.76	111.82
1	A	594	ARG	NE-CZ-NH1	-7.68	113.82	121.50
1	A	350	PHE	N-CA-C	-7.52	104.10	113.28
1	A	667	ASN	N-CA-C	-6.93	104.14	112.59
1	B	667	ASN	N-CA-C	-6.90	104.18	112.59
1	B	193	ARG	N-CA-C	6.85	119.41	110.43
1	A	193	ARG	N-CA-C	6.79	119.32	110.43
1	A	504	MET	N-CA-C	-6.79	98.18	109.24
1	A	292	GLY	N-CA-C	6.72	121.15	112.68
1	B	504	MET	N-CA-C	-6.67	98.38	109.24
1	A	510	SER	N-CA-C	6.35	124.33	110.80
1	A	245	GLU	N-CA-C	-6.32	105.56	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	GLU	N-CA-C	-6.25	105.65	113.28
1	B	510	SER	N-CA-C	6.18	123.97	110.80
1	B	39	LEU	N-CA-C	-6.14	104.70	111.82
1	A	626	THR	CA-C-N	-6.08	114.50	120.52
1	A	626	THR	C-N-CA	-6.08	114.50	120.52
1	B	292	GLY	N-CA-C	6.03	120.48	112.65
1	B	594	ARG	CG-CD-NE	5.98	125.17	112.00
1	B	462	GLU	N-CA-C	5.95	118.53	111.33
1	A	462	GLU	N-CA-C	5.93	118.51	111.33
1	A	39	LEU	N-CA-C	-5.92	104.96	111.82
1	B	429	ALA	CA-C-N	5.90	127.22	119.84
1	B	429	ALA	C-N-CA	5.90	127.22	119.84
1	A	316	LEU	CA-C-N	5.89	127.21	119.84
1	A	316	LEU	C-N-CA	5.89	127.21	119.84
1	B	626	THR	CA-C-N	-5.83	114.75	120.52
1	B	626	THR	C-N-CA	-5.83	114.75	120.52
1	B	612	ASP	N-CA-C	-5.81	103.04	110.53
1	A	686	GLN	CA-C-N	5.75	127.03	119.84
1	A	686	GLN	C-N-CA	5.75	127.03	119.84
1	B	686	GLN	CA-C-N	5.75	127.02	119.84
1	B	686	GLN	C-N-CA	5.75	127.02	119.84
1	B	594	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	B	627	PRO	N-CA-C	-5.72	102.61	111.13
1	A	266	ARG	N-CA-C	5.67	117.92	111.11
1	A	627	PRO	N-CA-C	-5.65	102.72	111.13
1	A	429	ALA	CA-C-N	5.61	126.85	119.84
1	A	429	ALA	C-N-CA	5.61	126.85	119.84
1	A	608	LEU	N-CA-C	-5.55	100.66	109.59
1	B	670	LYS	N-CA-C	-5.50	101.51	109.59
1	B	266	ARG	N-CA-C	5.49	117.70	111.11
1	A	413	HIS	N-CA-C	-5.47	105.73	112.90
1	B	202	ILE	N-CA-C	-5.43	105.24	110.72
1	B	608	LEU	N-CA-C	-5.41	100.36	109.07
1	B	413	HIS	N-CA-C	-5.41	105.82	112.90
1	B	316	LEU	CA-C-N	5.40	126.59	119.84
1	B	316	LEU	C-N-CA	5.40	126.59	119.84
1	B	546	VAL	N-CA-C	-5.39	105.47	110.53
1	A	250	SER	N-CA-C	-5.37	106.11	113.30
1	B	251	LEU	N-CA-C	-5.35	106.76	113.72
1	B	250	SER	N-CA-C	-5.35	106.13	113.30
1	A	612	ASP	N-CA-C	-5.33	103.65	110.53
1	A	251	LEU	N-CA-C	-5.32	106.81	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	670	LYS	N-CA-C	-5.15	102.01	109.59
1	B	476	ALA	N-CA-C	-5.14	105.76	113.89
1	B	609	SER	N-CA-C	5.13	116.99	109.24
1	A	493	ASN	CA-C-N	5.13	126.14	120.45
1	A	493	ASN	C-N-CA	5.13	126.14	120.45
1	B	493	ASN	CA-C-N	5.05	126.05	120.45
1	B	493	ASN	C-N-CA	5.05	126.05	120.45
1	A	258	GLU	CA-C-N	5.02	125.03	120.21
1	A	258	GLU	C-N-CA	5.02	125.03	120.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5671	0	5721	264	0
1	B	5671	0	5721	271	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	12	2	0
3	B	31	0	12	5	0
4	A	76	0	0	3	0
4	B	54	0	0	6	0
All	All	11538	0	11466	530	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 23.

All (530) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:HG3	1:A:251:LEU:HG	1.43	1.00
1:B:672:ARG:HD3	1:B:675:LEU:HD12	1.39	1.00
1:A:672:ARG:HD3	1:A:675:LEU:HD12	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:HG3	1:B:251:LEU:HG	1.45	0.99
1:A:193:ARG:HB3	1:A:195:PRO:HD3	1.54	0.90
1:A:277:ARG:HG2	1:A:282:ILE:HD12	1.54	0.88
1:B:193:ARG:HB3	1:B:195:PRO:HD3	1.54	0.88
1:B:277:ARG:HG2	1:B:282:ILE:HD12	1.56	0.87
1:A:435:HIS:NE2	3:A:701:ATP:O3G	2.09	0.85
1:B:53:ARG:HH12	1:B:566:MET:HE2	1.42	0.85
1:B:240:GLU:HB3	1:B:244:MET:HB2	1.60	0.84
1:A:53:ARG:HH12	1:A:566:MET:HE2	1.43	0.83
1:A:63:ILE:HG12	1:A:255:LEU:HD11	1.60	0.83
1:A:240:GLU:HB3	1:A:244:MET:HB2	1.60	0.83
1:B:179:VAL:HG13	1:B:180:PRO:HD2	1.61	0.81
1:A:426:ILE:HD13	1:A:492:GLU:HG2	1.63	0.81
1:B:63:ILE:HG12	1:B:255:LEU:HD11	1.60	0.81
1:A:402:LEU:HD22	1:A:427:PHE:HD2	1.43	0.81
1:B:402:LEU:HD22	1:B:427:PHE:HD2	1.46	0.81
1:A:141:ASN:HB3	1:A:142:PRO:HD2	1.63	0.81
1:B:141:ASN:HB3	1:B:142:PRO:HD2	1.63	0.80
1:B:413:HIS:C	1:B:415:ALA:H	1.89	0.80
1:A:344:TYR:H	1:A:348:HIS:HD2	1.25	0.80
1:B:116:SER:C	1:B:118:ASN:H	1.89	0.80
1:A:116:SER:C	1:A:118:ASN:H	1.89	0.80
1:A:594:ARG:HH21	1:A:610:SER:C	1.89	0.80
1:B:344:TYR:H	1:B:348:HIS:HD2	1.28	0.79
1:A:179:VAL:HG13	1:A:180:PRO:HD2	1.65	0.79
1:B:426:ILE:HD13	1:B:492:GLU:HG2	1.65	0.78
1:B:53:ARG:NH1	1:B:566:MET:HE2	2.00	0.77
3:B:704:ATP:H2'	3:B:704:ATP:N3	1.99	0.77
1:A:413:HIS:C	1:A:415:ALA:H	1.89	0.77
1:A:614:MET:HB2	1:A:617:ASN:ND2	2.00	0.76
1:B:244:MET:HA	1:B:247:MET:HB2	1.67	0.76
1:B:614:MET:HB2	1:B:617:ASN:ND2	2.00	0.76
1:B:403:GLN:HE22	1:B:430:PRO:HA	1.51	0.76
1:A:244:MET:HA	1:A:247:MET:HB2	1.68	0.76
1:B:594:ARG:HD3	1:B:612:ASP:OD1	1.87	0.75
1:A:111:ASN:H	1:A:114:GLN:HE21	1.36	0.74
1:A:403:GLN:HE22	1:A:430:PRO:HA	1.52	0.74
1:A:53:ARG:NH1	1:A:566:MET:HE2	2.03	0.73
1:A:61:ILE:HD13	1:A:73:SER:HB2	1.70	0.73
1:A:20:ARG:HG2	1:A:652:ARG:HD2	1.70	0.72
1:A:265:GLN:HE21	1:A:293:ARG:HA	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:H	1:B:114:GLN:HE21	1.37	0.72
1:B:61:ILE:HD13	1:B:73:SER:HB2	1.70	0.72
1:B:468:TYR:OH	3:B:704:ATP:O3'	2.08	0.72
1:B:20:ARG:HG2	1:B:652:ARG:HD2	1.70	0.72
1:A:22:LEU:HD22	1:A:94:LEU:HD12	1.71	0.71
1:B:437:LYS:HG2	1:B:458:GLY:O	1.89	0.71
1:B:265:GLN:HE21	1:B:293:ARG:HA	1.54	0.71
1:A:437:LYS:HG2	1:A:458:GLY:O	1.91	0.71
1:B:22:LEU:HD22	1:B:94:LEU:HD12	1.71	0.70
1:B:606:VAL:HG21	1:B:634:LYS:HG3	1.72	0.70
1:A:240:GLU:CB	1:A:244:MET:HB2	2.22	0.70
1:A:345:TYR:O	1:A:469:THR:HA	1.92	0.70
1:B:106:GLN:O	1:B:194:LYS:HB2	1.92	0.69
1:A:163:ARG:O	1:A:166:THR:HB	1.92	0.69
1:B:163:ARG:O	1:B:166:THR:HB	1.94	0.68
1:A:426:ILE:CD1	1:A:492:GLU:HG2	2.23	0.68
1:A:380:SER:HB3	1:A:383:ILE:HG12	1.77	0.67
1:B:33:ILE:HG12	1:B:311:LEU:HB3	1.76	0.67
1:A:106:GLN:O	1:A:194:LYS:HB2	1.95	0.67
1:B:240:GLU:CB	1:B:244:MET:HB2	2.22	0.67
1:B:265:GLN:NE2	1:B:293:ARG:HG3	2.10	0.67
1:A:265:GLN:NE2	1:A:293:ARG:HG3	2.09	0.67
1:A:370:LYS:HG2	1:A:397:THR:HB	1.77	0.67
1:B:288:ILE:HD12	1:B:288:ILE:N	2.10	0.67
1:B:426:ILE:CD1	1:B:492:GLU:HG2	2.25	0.67
1:A:72:HIS:HB3	1:A:75:HIS:CD2	2.30	0.66
1:A:33:ILE:HG12	1:A:311:LEU:HB3	1.76	0.66
1:B:72:HIS:HB3	1:B:75:HIS:CD2	2.31	0.66
1:A:139:LEU:HD11	1:B:362:PHE:O	1.96	0.66
1:B:370:LYS:HG2	1:B:397:THR:HB	1.78	0.65
1:B:59:ARG:O	1:B:63:ILE:HG13	1.97	0.65
1:A:288:ILE:HD12	1:A:288:ILE:N	2.12	0.65
1:B:23:GLN:OE1	1:B:652:ARG:HD3	1.97	0.65
1:B:345:TYR:O	1:B:469:THR:HA	1.96	0.65
1:A:59:ARG:O	1:A:63:ILE:HG13	1.96	0.65
1:A:363:ASP:OD2	1:A:443:ARG:NH1	2.30	0.64
1:A:53:ARG:NH1	1:A:566:MET:CE	2.59	0.64
1:B:380:SER:HB3	1:B:383:ILE:HG12	1.78	0.64
1:A:23:GLN:OE1	1:A:652:ARG:HD3	1.98	0.64
1:B:582:ALA:HB1	1:B:654:ILE:HD12	1.80	0.64
1:B:155:THR:O	1:B:174:ILE:HG12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:HB3	1:B:391:HIS:CE1	2.33	0.63
1:A:214:PHE:HZ	1:B:359:GLN:OE1	1.82	0.63
1:A:416:LYS:O	1:A:420:GLU:HB2	1.97	0.63
1:B:416:LYS:O	1:B:420:GLU:HB2	1.97	0.63
1:B:559:VAL:HB	1:B:580:ILE:HG12	1.81	0.63
1:A:614:MET:HB2	1:A:617:ASN:HD22	1.62	0.63
1:B:614:MET:HB2	1:B:617:ASN:HD22	1.62	0.63
1:A:155:THR:O	1:A:174:ILE:HG12	1.99	0.62
1:A:413:HIS:ND1	1:A:416:LYS:HE3	2.14	0.62
1:B:189:ALA:HB3	1:B:190:PRO:CD	2.28	0.62
1:B:363:ASP:OD2	1:B:443:ARG:NH1	2.32	0.62
1:A:189:ALA:HB3	1:A:190:PRO:CD	2.29	0.62
1:A:480:ILE:HD12	4:A:771:HOH:O	1.98	0.62
1:A:413:HIS:C	1:A:415:ALA:N	2.58	0.62
1:A:75:HIS:O	1:A:79:LYS:HG3	2.00	0.62
1:A:435:HIS:HE2	3:A:701:ATP:PG	2.22	0.62
1:A:548:ARG:HG2	1:A:548:ARG:HH11	1.64	0.61
1:A:322:ILE:HG23	4:A:753:HOH:O	2.00	0.61
1:A:606:VAL:HG21	1:A:634:LYS:HG3	1.80	0.61
1:B:75:HIS:O	1:B:79:LYS:HG3	2.00	0.61
1:B:371:ILE:HG13	1:B:439:PHE:HB3	1.83	0.61
1:A:207:LEU:HD11	1:A:222:ALA:HB2	1.82	0.61
1:A:559:VAL:HB	1:A:580:ILE:HG12	1.81	0.61
1:B:207:LEU:HD11	1:B:222:ALA:HB2	1.81	0.61
1:B:225:MET:HE2	1:B:276:LEU:HD13	1.81	0.61
1:B:413:HIS:ND1	1:B:416:LYS:HE3	2.16	0.61
1:A:225:MET:HE2	1:A:276:LEU:HD13	1.83	0.61
1:A:401:GLU:OE2	1:A:403:GLN:HB2	2.01	0.61
1:B:656:LYS:HG3	1:B:657:GLU:OE1	2.00	0.60
1:B:401:GLU:OE2	1:B:403:GLN:HB2	2.01	0.60
1:B:504:MET:HB3	1:B:625:ALA:HB3	1.82	0.60
1:B:606:VAL:CG2	1:B:634:LYS:HG3	2.31	0.60
1:A:247:MET:HE3	1:A:252:LYS:HB3	1.82	0.60
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.65	0.60
1:A:582:ALA:HB1	1:A:654:ILE:HD12	1.84	0.60
1:B:548:ARG:HG2	1:B:548:ARG:HH11	1.67	0.60
1:A:504:MET:HB3	1:A:625:ALA:HB3	1.83	0.60
1:B:72:HIS:HB3	1:B:75:HIS:HD2	1.67	0.60
1:A:72:HIS:HB3	1:A:75:HIS:HD2	1.67	0.59
1:A:111:ASN:H	1:A:114:GLN:NE2	1.99	0.59
1:B:53:ARG:NH1	1:B:566:MET:CE	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ILE:HG23	1:B:376:VAL:HG13	1.83	0.59
1:A:594:ARG:NH2	1:A:610:SER:O	2.34	0.59
1:A:373:ILE:HG23	1:A:376:VAL:HG13	1.84	0.59
1:B:247:MET:HE3	1:B:252:LYS:HB3	1.83	0.59
1:B:116:SER:O	1:B:120:GLN:HG3	2.03	0.59
1:B:147:VAL:HG22	1:B:279:LYS:O	2.03	0.59
1:B:111:ASN:H	1:B:114:GLN:NE2	2.01	0.59
1:B:536:LYS:HD3	1:B:562:LEU:HD23	1.85	0.59
1:A:116:SER:OG	1:A:119:GLN:HG3	2.03	0.59
1:A:656:LYS:HG3	1:A:657:GLU:OE1	2.03	0.58
1:B:26:ALA:HB2	1:B:94:LEU:HD11	1.85	0.58
1:B:594:ARG:NH2	1:B:610:SER:O	2.35	0.58
1:B:116:SER:O	1:B:118:ASN:N	2.37	0.58
1:A:323:TRP:HZ2	1:A:338:GLU:HG2	1.68	0.58
1:B:376:VAL:HG23	1:B:414:TRP:HE1	1.67	0.58
1:B:112:GLU:HB2	1:B:205:TYR:HB2	1.84	0.58
1:A:26:ALA:HB2	1:A:94:LEU:HD11	1.86	0.58
1:B:314:LYS:H	1:B:314:LYS:HD3	1.68	0.58
1:B:633:LEU:HD12	4:B:714:HOH:O	2.04	0.58
1:B:116:SER:OG	1:B:119:GLN:HG3	2.03	0.57
1:B:225:MET:HE1	1:B:276:LEU:HD22	1.86	0.57
1:A:225:MET:HE1	1:A:276:LEU:HD22	1.87	0.57
1:A:506:SER:O	1:A:622:ILE:HA	2.04	0.57
1:B:432:LEU:HD22	1:B:620:TYR:O	2.05	0.57
1:A:116:SER:O	1:A:120:GLN:HG3	2.04	0.57
1:A:314:LYS:H	1:A:314:LYS:HD3	1.67	0.57
1:A:432:LEU:HD22	1:A:620:TYR:O	2.05	0.57
1:A:116:SER:O	1:A:118:ASN:N	2.37	0.57
1:B:374:TYR:O	1:B:411:ASN:ND2	2.36	0.57
1:A:147:VAL:HG22	1:A:279:LYS:O	2.04	0.57
1:B:408:GLU:HG3	1:B:409:GLU:N	2.20	0.57
1:A:376:VAL:HG23	1:A:414:TRP:HE1	1.67	0.57
1:A:112:GLU:OE1	1:A:293:ARG:NH2	2.35	0.57
1:A:371:ILE:HG13	1:A:439:PHE:HB3	1.87	0.57
1:B:461:ASN:HB3	1:B:464:THR:HB	1.87	0.57
1:A:140:ILE:HD11	1:A:171:LEU:HG	1.86	0.56
1:B:323:TRP:HZ2	1:B:338:GLU:HG2	1.70	0.56
1:A:408:GLU:HG3	1:A:409:GLU:N	2.20	0.56
1:A:112:GLU:HB2	1:A:205:TYR:HB2	1.87	0.56
1:A:265:GLN:HE22	1:A:293:ARG:HG3	1.70	0.56
1:A:461:ASN:HB3	1:A:464:THR:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLU:HA	1:A:59:ARG:NH1	2.20	0.56
1:A:536:LYS:HD3	1:A:562:LEU:HD23	1.87	0.56
1:A:223:TYR:HA	1:A:265:GLN:OE1	2.05	0.56
1:A:374:TYR:O	1:A:411:ASN:ND2	2.38	0.56
1:B:140:ILE:HD11	1:B:171:LEU:HG	1.87	0.56
1:B:348:HIS:HE1	1:B:685:GLU:OE1	1.88	0.56
1:B:509:ASN:ND2	1:B:513:LEU:HD22	2.21	0.56
1:A:59:ARG:HD3	1:A:255:LEU:O	2.06	0.56
1:B:506:SER:O	1:B:622:ILE:HA	2.06	0.55
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.69	0.55
1:A:401:GLU:OE1	1:A:428:SER:HB2	2.07	0.55
1:B:112:GLU:OE1	1:B:293:ARG:NH2	2.36	0.55
1:B:56:GLU:HA	1:B:59:ARG:NH1	2.20	0.55
1:B:401:GLU:OE1	1:B:428:SER:HB2	2.07	0.55
1:A:348:HIS:HE1	1:A:685:GLU:OE1	1.90	0.55
1:B:267:ASP:O	1:B:268:MET:C	2.50	0.55
1:B:39:LEU:HD22	1:B:91:PHE:CE1	2.42	0.54
1:A:265:GLN:HE21	1:A:293:ARG:CA	2.21	0.54
1:A:432:LEU:HD11	1:A:622:ILE:HG13	1.89	0.54
1:B:265:GLN:HE21	1:B:293:ARG:CA	2.20	0.54
1:B:437:LYS:HG2	1:B:458:GLY:C	2.32	0.54
1:A:538:ASN:ND2	1:A:594:ARG:HH11	2.05	0.54
1:A:323:TRP:CZ2	1:A:338:GLU:HG2	2.42	0.54
1:A:414:TRP:HA	1:A:414:TRP:CE3	2.42	0.54
1:B:39:LEU:HD11	1:B:98:LEU:HD12	1.90	0.54
1:B:451:ARG:HB2	1:B:481:THR:CG2	2.37	0.54
1:B:455:ILE:HG21	1:B:626:THR:OG1	2.07	0.54
1:A:451:ARG:HB2	1:A:481:THR:CG2	2.38	0.54
1:B:223:TYR:HA	1:B:265:GLN:OE1	2.08	0.54
1:A:66:GLU:CG	1:A:251:LEU:HG	2.28	0.53
1:B:59:ARG:HH11	1:B:236:VAL:HG21	1.72	0.53
1:B:432:LEU:HD11	1:B:622:ILE:HG13	1.90	0.53
1:A:120:GLN:HB3	1:A:205:TYR:OH	2.09	0.53
1:A:267:ASP:O	1:A:268:MET:C	2.50	0.53
1:B:265:GLN:HE22	1:B:293:ARG:HG3	1.71	0.53
1:A:4:GLU:O	1:A:5:LYS:C	2.51	0.53
1:B:59:ARG:HD3	1:B:255:LEU:O	2.06	0.53
1:B:263:VAL:HA	1:B:289:VAL:O	2.09	0.53
1:B:644:LEU:HD23	1:B:673:ALA:HB1	1.91	0.53
1:A:414:TRP:HA	1:A:414:TRP:HE3	1.73	0.53
1:B:592:HIS:CE1	1:B:594:ARG:HH12	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:TRP:HA	1:B:414:TRP:CE3	2.43	0.53
1:B:414:TRP:HA	1:B:414:TRP:HE3	1.74	0.53
1:A:116:SER:HG	1:A:119:GLN:HG3	1.73	0.53
1:A:425:VAL:HG12	1:A:426:ILE:N	2.24	0.53
1:A:644:LEU:HD23	1:A:673:ALA:HB1	1.90	0.53
1:B:4:GLU:O	1:B:5:LYS:C	2.51	0.53
1:A:455:ILE:HG21	1:A:626:THR:OG1	2.09	0.53
1:B:117:VAL:HG12	1:B:117:VAL:O	2.09	0.53
1:B:271:ALA:O	1:B:275:VAL:HG23	2.08	0.53
1:A:22:LEU:CD2	1:A:94:LEU:HD12	2.39	0.53
1:A:468:TYR:N	1:A:468:TYR:CD1	2.77	0.53
1:A:509:ASN:ND2	1:A:513:LEU:HD22	2.23	0.53
1:B:520:ARG:HH11	1:B:605:LYS:HZ3	1.57	0.53
1:A:39:LEU:HD22	1:A:91:PHE:CE1	2.43	0.53
1:B:382:ILE:CD1	1:B:460:PHE:HB3	2.39	0.53
1:B:569:LEU:HD23	1:B:569:LEU:C	2.34	0.53
1:A:117:VAL:HG12	1:A:117:VAL:O	2.09	0.52
1:B:408:GLU:HG3	1:B:409:GLU:H	1.74	0.52
1:A:116:SER:C	1:A:118:ASN:N	2.58	0.52
1:A:263:VAL:HA	1:A:289:VAL:O	2.09	0.52
1:A:315:PRO:O	1:A:317:PRO:HD3	2.09	0.52
1:A:468:TYR:N	1:A:468:TYR:HD1	2.07	0.52
1:B:22:LEU:CD2	1:B:94:LEU:HD12	2.38	0.52
1:B:24:GLU:HB3	1:B:38:PHE:CE1	2.43	0.52
1:B:181:ARG:HD2	1:B:299:ASP:OD2	2.10	0.52
1:B:688:GLU:HG3	4:B:754:HOH:O	2.08	0.52
1:A:59:ARG:HH11	1:A:236:VAL:HG21	1.72	0.52
1:A:600:ASN:CG	1:A:605:LYS:HZ2	2.17	0.52
1:A:606:VAL:CG2	1:A:634:LYS:HG3	2.38	0.52
1:B:265:GLN:NE2	1:B:293:ARG:HA	2.22	0.52
1:B:509:ASN:HD22	1:B:513:LEU:HD22	1.74	0.52
1:A:149:PHE:CB	1:B:391:HIS:CE1	2.93	0.52
1:A:163:ARG:HG3	1:A:216:ASP:O	2.09	0.52
1:B:163:ARG:HG3	1:B:216:ASP:O	2.09	0.52
1:B:277:ARG:HA	1:B:282:ILE:HD12	1.92	0.52
1:B:323:TRP:CZ2	1:B:338:GLU:HG2	2.44	0.52
1:A:56:GLU:HA	1:A:59:ARG:HH12	1.75	0.51
1:B:358:ARG:NH2	4:B:739:HOH:O	2.43	0.51
1:B:79:LYS:O	1:B:82:SER:HB3	2.09	0.51
1:A:8:ILE:HD13	1:A:658:LEU:HD21	1.91	0.51
1:B:379:ASP:HA	1:B:414:TRP:CH2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:GLU:OE2	1:B:486:ARG:NH2	2.44	0.51
1:A:194:LYS:HB3	1:A:306:VAL:HG11	1.92	0.51
1:A:408:GLU:HG3	1:A:409:GLU:H	1.74	0.51
1:B:145:ASP:CG	1:B:145:ASP:O	2.54	0.51
1:A:382:ILE:CD1	1:A:460:PHE:HB3	2.40	0.51
1:B:468:TYR:HD1	1:B:468:TYR:N	2.09	0.51
1:A:277:ARG:HA	1:A:282:ILE:HD12	1.93	0.51
1:A:435:HIS:HB3	1:A:623:GLU:OE1	2.10	0.51
1:B:282:ILE:HG21	1:B:288:ILE:HD11	1.93	0.51
1:B:425:VAL:HG12	1:B:426:ILE:N	2.25	0.51
1:B:480:ILE:HD12	4:B:730:HOH:O	2.11	0.51
1:A:145:ASP:HB2	1:A:147:VAL:HG23	1.92	0.51
1:B:468:TYR:N	1:B:468:TYR:CD1	2.78	0.51
1:A:61:ILE:O	1:A:65:GLU:HG3	2.11	0.51
1:B:163:ARG:HG2	1:B:217:TYR:HA	1.93	0.51
1:A:437:LYS:HG2	1:A:458:GLY:C	2.35	0.50
1:A:553:SER:HB2	1:A:580:ILE:HG13	1.93	0.50
1:B:120:GLN:HB3	1:B:205:TYR:OH	2.11	0.50
1:B:594:ARG:HH21	1:B:610:SER:C	2.19	0.50
1:A:79:LYS:O	1:A:82:SER:HB3	2.10	0.50
1:A:108:PHE:CZ	1:A:193:ARG:NH1	2.79	0.50
1:A:282:ILE:HG21	1:A:288:ILE:HD11	1.93	0.50
1:B:145:ASP:HB2	1:B:147:VAL:HG23	1.93	0.50
1:B:8:ILE:HD13	1:B:658:LEU:HD21	1.92	0.50
1:B:22:LEU:HD22	1:B:94:LEU:CD1	2.41	0.50
1:B:56:GLU:HA	1:B:59:ARG:HH12	1.75	0.50
1:B:194:LYS:HB3	1:B:306:VAL:HG11	1.92	0.50
1:B:553:SER:HB2	1:B:580:ILE:HG13	1.93	0.50
1:A:379:ASP:HA	1:A:414:TRP:CH2	2.47	0.50
1:A:657:GLU:OE1	1:A:657:GLU:N	2.42	0.50
1:B:454:HIS:HA	1:B:473:LEU:O	2.12	0.50
1:A:24:GLU:HB3	1:A:38:PHE:CE1	2.46	0.50
1:A:145:ASP:CG	1:A:145:ASP:O	2.54	0.50
1:B:20:ARG:CG	1:B:652:ARG:HD2	2.41	0.50
1:B:402:LEU:HD22	1:B:427:PHE:CD2	2.37	0.50
1:B:589:TYR:HB2	1:B:674:GLN:NE2	2.27	0.50
1:A:285:TYR:HD1	1:A:285:TYR:H	1.58	0.50
1:A:454:HIS:HA	1:A:473:LEU:O	2.12	0.50
1:B:315:PRO:O	1:B:317:PRO:HD3	2.11	0.50
1:B:504:MET:HG3	1:B:513:LEU:HD23	1.94	0.50
1:B:594:ARG:HB2	1:B:609:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:PHE:CZ	1:B:193:ARG:NH1	2.80	0.50
1:A:589:TYR:HB2	1:A:674:GLN:NE2	2.27	0.49
1:B:59:ARG:HB3	1:B:255:LEU:HD22	1.94	0.49
1:B:665:ARG:O	1:B:665:ARG:HG3	2.10	0.49
1:B:66:GLU:CG	1:B:251:LEU:HG	2.29	0.49
1:B:83:ARG:H	1:B:83:ARG:HD2	1.77	0.49
1:B:116:SER:C	1:B:118:ASN:N	2.58	0.49
1:B:228:THR:HG22	1:B:229:ARG:N	2.26	0.49
1:A:39:LEU:HD11	1:A:98:LEU:HD12	1.93	0.49
1:A:163:ARG:HG2	1:A:217:TYR:HA	1.93	0.49
1:A:265:GLN:NE2	1:A:293:ARG:HA	2.22	0.49
1:B:61:ILE:O	1:B:65:GLU:HG3	2.12	0.49
1:B:439:PHE:CD1	1:B:439:PHE:C	2.90	0.49
1:B:189:ALA:HB3	1:B:190:PRO:HD3	1.94	0.49
1:B:288:ILE:HD12	1:B:288:ILE:H	1.77	0.49
1:B:587:ASP:CG	1:B:588:ARG:H	2.19	0.49
1:A:181:ARG:HD2	1:A:299:ASP:OD2	2.11	0.49
1:A:228:THR:HG22	1:A:229:ARG:N	2.26	0.49
1:A:251:LEU:O	1:A:255:LEU:HB2	2.13	0.49
1:A:59:ARG:HB3	1:A:255:LEU:HD22	1.93	0.49
1:A:271:ALA:O	1:A:275:VAL:HG23	2.12	0.49
1:B:285:TYR:HD1	1:B:285:TYR:H	1.59	0.49
1:B:314:LYS:H	1:B:314:LYS:CD	2.24	0.49
1:A:439:PHE:CD1	1:A:439:PHE:C	2.91	0.49
1:A:665:ARG:O	1:A:665:ARG:HG3	2.10	0.49
1:B:251:LEU:O	1:B:255:LEU:HB2	2.13	0.49
1:A:131:LEU:O	1:A:132:ARG:C	2.56	0.48
1:A:587:ASP:CG	1:A:588:ARG:H	2.21	0.48
1:A:251:LEU:CD2	1:A:255:LEU:HG	2.43	0.48
1:A:77:LEU:N	1:A:77:LEU:HD22	2.28	0.48
1:B:251:LEU:CD2	1:B:255:LEU:HG	2.43	0.48
1:A:22:LEU:HD22	1:A:94:LEU:CD1	2.42	0.48
1:B:468:TYR:OH	3:B:704:ATP:H3'	2.13	0.48
1:B:657:GLU:OE1	1:B:657:GLU:N	2.44	0.48
1:A:504:MET:HG3	1:A:513:LEU:HD23	1.96	0.48
1:B:435:HIS:HB3	1:B:623:GLU:OE1	2.14	0.48
1:A:569:LEU:C	1:A:569:LEU:HD23	2.38	0.48
1:B:77:LEU:N	1:B:77:LEU:HD22	2.29	0.48
1:A:169:TYR:CE2	1:A:272:LEU:HG	2.49	0.48
1:A:437:LYS:HE3	1:A:459:ASN:HB3	1.96	0.48
1:B:169:TYR:CE2	1:B:272:LEU:HG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:CG	1:A:652:ARG:HD2	2.42	0.48
1:A:402:LEU:HD22	1:A:427:PHE:CD2	2.35	0.47
1:A:509:ASN:HD22	1:A:513:LEU:HD22	1.78	0.47
1:A:537:LEU:HA	1:A:594:ARG:HG2	1.96	0.47
1:A:146:LEU:O	1:A:147:VAL:C	2.57	0.47
1:B:539:ASN:ND2	1:B:566:MET:H	2.12	0.47
1:A:538:ASN:HD22	1:A:594:ARG:HH11	1.62	0.47
1:A:111:ASN:N	1:A:114:GLN:HE21	2.10	0.47
1:A:314:LYS:H	1:A:314:LYS:CD	2.24	0.47
1:A:536:LYS:O	1:A:594:ARG:HA	2.15	0.47
1:A:539:ASN:ND2	1:A:566:MET:H	2.13	0.47
1:A:105:ASN:O	1:A:106:GLN:HB2	2.14	0.47
1:B:179:VAL:HG13	1:B:180:PRO:CD	2.39	0.47
1:A:189:ALA:HB3	1:A:190:PRO:HD3	1.96	0.47
1:B:102:MET:HB3	1:B:107:ILE:HB	1.96	0.47
1:B:105:ASN:O	1:B:106:GLN:HB2	2.14	0.47
1:B:179:VAL:CG1	1:B:180:PRO:HD2	2.39	0.47
1:B:20:ARG:NH2	4:B:750:HOH:O	2.47	0.47
1:A:288:ILE:HD12	1:A:288:ILE:H	1.79	0.47
1:A:498:VAL:HG12	1:A:499:THR:N	2.29	0.47
1:A:659:SER:OG	1:A:661:ARG:HG3	2.15	0.47
1:A:539:ASN:HD22	1:A:566:MET:H	1.63	0.47
1:B:131:LEU:O	1:B:132:ARG:C	2.58	0.47
1:A:161:ILE:HB	1:A:168:ARG:HB2	1.96	0.46
1:A:61:ILE:CD1	1:A:77:LEU:HD21	2.46	0.46
1:A:77:LEU:HD22	1:A:77:LEU:H	1.80	0.46
1:A:284:ARG:HG3	1:A:285:TYR:N	2.30	0.46
1:A:413:HIS:O	1:A:415:ALA:N	2.47	0.46
1:B:564:ARG:HG3	1:B:565:GLY:N	2.30	0.46
1:A:680:TYR:O	1:A:683:SER:HB3	2.16	0.46
1:B:225:MET:CE	1:B:276:LEU:HD13	2.46	0.46
1:A:483:GLU:OE2	1:A:486:ARG:NH2	2.48	0.46
1:B:161:ILE:HB	1:B:168:ARG:HB2	1.98	0.46
1:A:464:THR:C	1:A:466:ARG:H	2.24	0.46
1:B:400:VAL:HG23	1:B:400:VAL:O	2.16	0.46
1:A:400:VAL:O	1:A:400:VAL:HG23	2.16	0.46
1:A:401:GLU:C	1:A:403:GLN:H	2.24	0.46
1:A:411:ASN:HA	1:A:414:TRP:HB2	1.98	0.46
1:B:451:ARG:HB2	1:B:481:THR:HG21	1.96	0.46
1:A:235:LEU:HD21	1:A:433:LYS:NZ	2.31	0.45
1:A:350:PHE:HB2	1:A:465:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ARG:HG3	1:B:285:TYR:N	2.31	0.45
1:A:63:ILE:HG13	1:A:255:LEU:HD21	1.97	0.45
1:A:355:GLU:HG2	1:B:132:ARG:NH1	2.31	0.45
1:A:451:ARG:HB2	1:A:481:THR:HG21	1.97	0.45
1:A:542:ASP:O	1:A:546:VAL:HG23	2.16	0.45
1:B:63:ILE:HG13	1:B:255:LEU:HD21	1.97	0.45
1:B:413:HIS:O	1:B:415:ALA:N	2.48	0.45
1:B:63:ILE:CG1	1:B:255:LEU:HD11	2.40	0.45
1:B:373:ILE:HG23	1:B:376:VAL:CG1	2.46	0.45
1:B:61:ILE:CD1	1:B:77:LEU:HD21	2.46	0.45
1:B:77:LEU:HD22	1:B:77:LEU:H	1.81	0.45
1:B:194:LYS:N	1:B:195:PRO:CD	2.79	0.45
1:B:437:LYS:HG3	1:B:459:ASN:HA	1.97	0.45
1:B:498:VAL:HG12	1:B:499:THR:N	2.31	0.45
1:A:323:TRP:CZ2	1:A:329:PHE:HZ	2.34	0.45
1:B:146:LEU:O	1:B:147:VAL:C	2.59	0.45
1:B:326:LYS:HE2	1:B:688:GLU:OE2	2.16	0.45
1:A:83:ARG:H	1:A:83:ARG:HD2	1.81	0.45
1:A:225:MET:CE	1:A:276:LEU:HD13	2.46	0.45
1:A:435:HIS:O	1:A:437:LYS:HD2	2.16	0.45
1:A:179:VAL:HG13	1:A:180:PRO:CD	2.42	0.45
1:A:437:LYS:HG3	1:A:459:ASN:HA	1.98	0.45
1:A:577:SER:HB2	1:A:580:ILE:HD12	1.98	0.45
1:A:615:THR:HG22	1:A:620:TYR:HE1	1.82	0.45
1:A:12:LEU:HD11	1:A:79:LYS:HD2	1.98	0.45
1:A:482:ASN:O	1:A:485:ARG:HB3	2.16	0.45
1:B:190:PRO:HG2	1:B:193:ARG:HD3	1.99	0.45
1:B:539:ASN:HD22	1:B:566:MET:H	1.63	0.45
1:A:363:ASP:CG	1:B:214:PHE:CD2	2.95	0.45
1:B:59:ARG:HB3	1:B:255:LEU:CD2	2.47	0.45
1:B:411:ASN:HA	1:B:414:TRP:HB2	1.98	0.45
1:A:194:LYS:N	1:A:195:PRO:CD	2.80	0.44
1:A:59:ARG:HB3	1:A:255:LEU:CD2	2.46	0.44
1:A:63:ILE:CG1	1:A:255:LEU:HD11	2.39	0.44
1:A:79:LYS:O	1:A:83:ARG:HD2	2.17	0.44
1:B:116:SER:HG	1:B:119:GLN:HG3	1.81	0.44
1:B:350:PHE:HB2	1:B:465:ALA:HB1	1.99	0.44
1:B:680:TYR:O	1:B:683:SER:HB3	2.16	0.44
1:A:467:LEU:C	1:A:468:TYR:HD1	2.25	0.44
1:B:437:LYS:HE3	1:B:459:ASN:HB3	2.00	0.44
1:B:468:TYR:OH	3:B:704:ATP:C3'	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:ASN:O	1:B:485:ARG:HB3	2.17	0.44
1:B:564:ARG:CZ	1:B:590:LEU:HD21	2.48	0.44
1:A:58:LYS:O	1:A:62:ILE:HG13	2.18	0.44
1:A:344:TYR:H	1:A:348:HIS:CD2	2.16	0.44
1:B:249:SER:HB2	1:B:252:LYS:HE2	1.99	0.44
1:B:354:LEU:HD13	1:B:381:ARG:CZ	2.47	0.44
1:A:102:MET:HB3	1:A:107:ILE:HB	2.00	0.44
1:A:375:ARG:NH2	1:A:405:ARG:HB2	2.33	0.44
1:A:120:GLN:HB3	1:A:205:TYR:CZ	2.53	0.44
1:A:244:MET:HG3	1:A:247:MET:SD	2.58	0.44
1:B:108:PHE:CD1	1:B:108:PHE:N	2.86	0.44
1:B:435:HIS:O	1:B:437:LYS:HD2	2.17	0.44
1:B:264:TYR:HE1	1:B:288:ILE:HG22	1.83	0.43
1:B:398:VAL:HG12	1:B:400:VAL:CG1	2.48	0.43
1:A:249:SER:HB2	1:A:252:LYS:HE2	1.99	0.43
1:B:296:ASN:OD1	1:B:298:LYS:HE2	2.18	0.43
1:A:564:ARG:HG3	1:A:565:GLY:N	2.31	0.43
1:B:557:VAL:HA	1:B:558:PRO:HD3	1.89	0.43
1:A:373:ILE:HG23	1:A:376:VAL:CG1	2.47	0.43
1:A:594:ARG:HB2	1:A:609:SER:O	2.18	0.43
1:B:150:LEU:HD12	1:B:150:LEU:HA	1.78	0.43
1:B:223:TYR:CZ	1:B:269:PRO:HD3	2.53	0.43
1:B:235:LEU:HD21	1:B:433:LYS:NZ	2.33	0.43
1:B:244:MET:HG3	1:B:247:MET:SD	2.58	0.43
1:B:12:LEU:HD11	1:B:79:LYS:HD2	2.00	0.43
1:B:83:ARG:HG2	1:B:83:ARG:NH1	2.32	0.43
1:B:120:GLN:HB3	1:B:205:TYR:CZ	2.53	0.43
1:B:611:ALA:HB2	1:B:623:GLU:HB3	2.00	0.43
1:A:36:MET:HE2	1:A:102:MET:HE1	2.01	0.43
1:A:464:THR:C	1:A:466:ARG:N	2.76	0.43
1:B:401:GLU:C	1:B:403:GLN:H	2.25	0.43
1:B:477:ASP:OD1	1:B:479:ARG:HD3	2.18	0.43
1:B:628:LEU:HA	4:B:722:HOH:O	2.19	0.43
1:A:564:ARG:CZ	1:A:590:LEU:HD21	2.48	0.43
1:B:36:MET:HE2	1:B:102:MET:HE1	2.00	0.43
1:B:46:LEU:O	1:B:49:PHE:HB3	2.18	0.43
1:B:266:ARG:HH11	1:B:266:ARG:HG2	1.84	0.43
1:B:458:GLY:HA3	1:B:470:ASP:CG	2.44	0.43
1:B:615:THR:HG22	1:B:620:TYR:HE1	1.83	0.43
1:A:534:THR:HB	1:A:597:ILE:HB	2.00	0.43
1:B:123:LEU:HD23	1:B:123:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ARG:NH2	1:B:405:ARG:HB2	2.34	0.43
1:B:467:LEU:C	1:B:468:TYR:HD1	2.27	0.43
1:B:542:ASP:O	1:B:546:VAL:HG23	2.19	0.43
1:A:108:PHE:CD1	1:A:108:PHE:N	2.86	0.43
1:B:58:LYS:O	1:B:62:ILE:HG13	2.19	0.43
1:B:345:TYR:HB3	1:B:346:PRO:HA	2.01	0.43
1:B:372:ASN:HD22	1:B:438:LEU:H	1.67	0.43
1:B:464:THR:C	1:B:466:ARG:H	2.27	0.42
1:B:659:SER:OG	1:B:661:ARG:HG3	2.19	0.42
1:B:233:TYR:CE1	1:B:236:VAL:HB	2.54	0.42
1:A:223:TYR:CZ	1:A:269:PRO:HD3	2.54	0.42
1:B:349:THR:CG2	1:B:351:GLU:HB2	2.50	0.42
1:B:520:ARG:NH1	1:B:605:LYS:HZ3	2.16	0.42
1:A:312:VAL:HG21	4:A:734:HOH:O	2.19	0.42
1:A:345:TYR:HB3	1:A:346:PRO:HA	2.00	0.42
1:A:372:ASN:HD22	1:A:438:LEU:H	1.67	0.42
1:A:179:VAL:CG1	1:A:180:PRO:HD2	2.42	0.42
1:A:233:TYR:CE1	1:A:236:VAL:HB	2.54	0.42
1:A:458:GLY:HA3	1:A:470:ASP:CG	2.45	0.42
1:B:618:ILE:HD12	1:B:618:ILE:N	2.34	0.42
1:A:296:ASN:OD1	1:A:298:LYS:HE2	2.19	0.42
1:A:354:LEU:HD13	1:A:381:ARG:CZ	2.50	0.42
1:A:477:ASP:OD1	1:A:479:ARG:HD3	2.19	0.42
1:B:318:ARG:CZ	1:B:466:ARG:HG2	2.50	0.42
1:B:594:ARG:CD	1:B:612:ASP:OD1	2.63	0.42
1:A:87:ALA:HA	1:A:90:GLU:OE1	2.19	0.42
1:A:398:VAL:HG12	1:A:400:VAL:CG1	2.48	0.42
1:B:87:ALA:HA	1:B:90:GLU:OE1	2.20	0.42
1:A:77:LEU:H	1:A:77:LEU:CD2	2.32	0.41
1:B:77:LEU:H	1:B:77:LEU:CD2	2.33	0.41
1:B:323:TRP:CZ2	1:B:329:PHE:HZ	2.38	0.41
1:A:63:ILE:HA	1:A:251:LEU:HD21	2.02	0.41
1:A:611:ALA:HB2	1:A:623:GLU:HB3	2.02	0.41
1:B:261:ARG:HE	1:B:261:ARG:HB3	1.75	0.41
1:B:648:THR:HB	1:B:665:ARG:HB3	2.01	0.41
1:B:158:ALA:HA	1:B:171:LEU:HD23	2.02	0.41
1:A:264:TYR:HE1	1:A:288:ILE:HG22	1.84	0.41
1:A:451:ARG:HB2	1:A:481:THR:HG23	2.02	0.41
1:A:498:VAL:CG1	1:A:499:THR:N	2.83	0.41
1:B:79:LYS:O	1:B:83:ARG:HD2	2.18	0.41
1:A:233:TYR:CD1	1:A:236:VAL:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:HIS:ND1	1:A:454:HIS:C	2.78	0.41
1:B:379:ASP:HA	1:B:414:TRP:HH2	1.83	0.41
1:B:451:ARG:HB2	1:B:481:THR:HG23	2.01	0.41
1:A:206:CYS:O	1:A:207:LEU:C	2.62	0.41
1:B:264:TYR:CE1	1:B:288:ILE:HG22	2.55	0.41
1:A:46:LEU:O	1:A:49:PHE:HB3	2.21	0.41
1:A:648:THR:HB	1:A:665:ARG:HB3	2.03	0.41
1:B:125:HIS:CE1	1:B:129:GLN:HG3	2.56	0.41
1:B:398:VAL:HG12	1:B:400:VAL:HG13	2.03	0.41
1:B:402:LEU:HD23	1:B:403:GLN:HG3	2.01	0.41
1:B:534:THR:HB	1:B:597:ILE:HB	2.02	0.41
1:B:536:LYS:O	1:B:594:ARG:HA	2.21	0.41
1:B:564:ARG:NE	1:B:590:LEU:HD21	2.35	0.41
1:A:190:PRO:HG2	1:A:193:ARG:HD3	2.03	0.41
1:A:326:LYS:HE2	1:A:688:GLU:OE2	2.20	0.41
1:B:454:HIS:ND1	1:B:454:HIS:C	2.79	0.41
1:B:590:LEU:HD11	3:B:704:ATP:H5'2	2.02	0.41
1:A:235:LEU:CD2	1:A:433:LYS:HZ1	2.34	0.40
1:A:251:LEU:HD23	1:A:255:LEU:HG	2.03	0.40
1:A:437:LYS:HE3	1:A:459:ASN:CA	2.51	0.40
1:A:546:VAL:HG12	1:A:550:TYR:CE1	2.56	0.40
1:B:233:TYR:CD1	1:B:236:VAL:HB	2.55	0.40
1:A:322:ILE:HD13	1:A:322:ILE:HA	1.80	0.40
1:B:616:ARG:HA	1:B:620:TYR:HD1	1.86	0.40
1:A:264:TYR:CE1	1:A:288:ILE:HG22	2.56	0.40
1:A:402:LEU:HD23	1:A:403:GLN:HG3	2.03	0.40
1:A:131:LEU:HD21	1:A:179:VAL:HG11	2.03	0.40
1:A:223:TYR:HE2	1:A:267:ASP:HB2	1.87	0.40
1:B:272:LEU:HD22	1:B:276:LEU:HD11	2.03	0.40
1:B:413:HIS:C	1:B:415:ALA:N	2.58	0.40
1:A:9:GLU:H	1:A:9:GLU:HG2	1.68	0.40
1:A:83:ARG:HG2	1:A:83:ARG:NH1	2.35	0.40
1:A:375:ARG:HH22	1:A:405:ARG:HD2	1.87	0.40
1:B:66:GLU:HG2	1:B:254:ARG:HH11	1.86	0.40
1:B:435:HIS:HE1	1:B:594:ARG:HH22	1.69	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	685/687 (100%)	623 (91%)	47 (7%)	15 (2%)	5	9
1	B	685/687 (100%)	626 (91%)	44 (6%)	15 (2%)	5	9
All	All	1370/1374 (100%)	1249 (91%)	91 (7%)	30 (2%)	5	9

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	ALA
1	A	430	PRO
1	A	510	SER
1	B	189	ALA
1	B	430	PRO
1	B	510	SER
1	A	117	VAL
1	A	147	VAL
1	A	148	GLN
1	B	117	VAL
1	B	147	VAL
1	B	148	GLN
1	A	5	LYS
1	A	149	PHE
1	A	233	TYR
1	A	283	SER
1	A	414	TRP
1	A	666	GLY
1	B	5	LYS
1	B	149	PHE
1	B	233	TYR
1	B	283	SER
1	B	414	TRP
1	B	666	GLY
1	A	404	ALA

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Mol	Chain	Res	Type
1	A	687	PRO
1	B	404	ALA
1	B	687	PRO
1	A	673	ALA
1	B	673	ALA

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	619/619 (100%)	573 (93%)	46 (7%)	13	27
1	B	619/619 (100%)	574 (93%)	45 (7%)	13	27
All	All	1238/1238 (100%)	1147 (93%)	91 (7%)	13	27

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	66	GLU
1	A	143	ASP
1	A	147	VAL
1	A	157	LEU
1	A	166	THR
1	A	177	ASP
1	A	196	MET
1	A	225	MET
1	A	230	ASP
1	A	234	ASP
1	A	244	MET
1	A	251	LEU
1	A	253	GLN
1	A	267	ASP
1	A	272	LEU
1	A	285	TYR
1	A	288	ILE

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Mol	Chain	Res	Type
1	A	314	LYS
1	A	322	ILE
1	A	343	LEU
1	A	349	THR
1	A	356	LEU
1	A	384	ASP
1	A	406	PHE
1	A	414	TRP
1	A	417	ARG
1	A	424	HIS
1	A	430	PRO
1	A	434	ILE
1	A	439	PHE
1	A	464	THR
1	A	468	TYR
1	A	472	SER
1	A	474	LEU
1	A	479	ARG
1	A	481	THR
1	A	496	ARG
1	A	564	ARG
1	A	590	LEU
1	A	595	VAL
1	A	616	ARG
1	A	626	THR
1	A	656	LYS
1	A	668	ARG
1	A	687	PRO
1	B	22	LEU
1	B	66	GLU
1	B	143	ASP
1	B	147	VAL
1	B	157	LEU
1	B	166	THR
1	B	177	ASP
1	B	196	MET
1	B	225	MET
1	B	230	ASP
1	B	234	ASP
1	B	244	MET
1	B	251	LEU
1	B	253	GLN

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Mol	Chain	Res	Type
1	B	267	ASP
1	B	272	LEU
1	B	285	TYR
1	B	288	ILE
1	B	314	LYS
1	B	322	ILE
1	B	343	LEU
1	B	349	THR
1	B	356	LEU
1	B	384	ASP
1	B	406	PHE
1	B	414	TRP
1	B	424	HIS
1	B	430	PRO
1	B	434	ILE
1	B	439	PHE
1	B	464	THR
1	B	468	TYR
1	B	472	SER
1	B	474	LEU
1	B	479	ARG
1	B	481	THR
1	B	496	ARG
1	B	564	ARG
1	B	590	LEU
1	B	595	VAL
1	B	616	ARG
1	B	626	THR
1	B	656	LYS
1	B	668	ARG
1	B	687	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	114	GLN
1	A	121	ASN
1	A	125	HIS
1	A	253	GLN
1	A	265	GLN
1	A	313	ASN

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Mol	Chain	Res	Type
1	A	328	GLN
1	A	348	HIS
1	A	391	HIS
1	A	403	GLN
1	A	446	ASN
1	A	509	ASN
1	A	526	GLN
1	A	527	GLN
1	A	539	ASN
1	A	560	ASN
1	A	617	ASN
1	B	75	HIS
1	B	114	GLN
1	B	121	ASN
1	B	125	HIS
1	B	253	GLN
1	B	265	GLN
1	B	313	ASN
1	B	328	GLN
1	B	348	HIS
1	B	403	GLN
1	B	424	HIS
1	B	446	ASN
1	B	509	ASN
1	B	526	GLN
1	B	527	GLN
1	B	539	ASN
1	B	560	ASN
1	B	617	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	704	2	32,33,33	2.87	13 (40%)	48,52,52	3.32	17 (35%)
3	ATP	A	701	2	32,33,33	4.19	20 (62%)	48,52,52	3.44	20 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	704	2	-	4/22/38/38	0/3/3/3
3	ATP	A	701	2	-	6/22/38/38	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ATP	PB-O3A	16.32	1.77	1.59
3	B	704	ATP	PB-O3A	10.75	1.71	1.59
3	A	701	ATP	C4-N3	7.52	1.48	1.34
3	A	701	ATP	O5'-C5'	-6.92	1.18	1.44
3	B	704	ATP	C4-N3	5.48	1.44	1.34
3	A	701	ATP	PB-O3B	4.87	1.64	1.59
3	B	704	ATP	O4'-C1'	4.49	1.52	1.42
3	A	701	ATP	C3'-C4'	-4.42	1.41	1.53
3	A	701	ATP	C8-N9	4.29	1.44	1.37
3	A	701	ATP	PA-O3A	4.07	1.63	1.59
3	A	701	ATP	C2'-C1'	3.99	1.66	1.53
3	A	701	ATP	C5-C6	3.35	1.50	1.41
3	B	704	ATP	O5'-C5'	-3.32	1.32	1.44
3	A	701	ATP	C1'-N9	3.24	1.55	1.46
3	B	704	ATP	C8-N9	3.21	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	704	ATP	C6-N1	3.21	1.44	1.35
3	A	701	ATP	O4'-C1'	3.07	1.49	1.42
3	B	704	ATP	C5-C6	3.06	1.49	1.41
3	A	701	ATP	O4'-C4'	2.96	1.51	1.45
3	B	704	ATP	O4'-C4'	2.79	1.51	1.45
3	A	701	ATP	C2-N3	2.76	1.38	1.33
3	B	704	ATP	PB-O3B	2.75	1.62	1.59
3	A	701	ATP	C2'-C3'	2.57	1.60	1.53
3	B	704	ATP	C5-N7	2.53	1.43	1.39
3	A	701	ATP	PG-O1G	2.49	1.58	1.50
3	B	704	ATP	PA-O3A	-2.44	1.56	1.59
3	A	701	ATP	C4-N9	2.33	1.42	1.37
3	A	701	ATP	C6-N1	2.30	1.42	1.35
3	A	701	ATP	C6-N6	2.30	1.40	1.34
3	A	701	ATP	PA-O2A	2.28	1.65	1.55
3	B	704	ATP	C5'-C4'	-2.15	1.45	1.51
3	A	701	ATP	O3'-C3'	2.10	1.48	1.43
3	B	704	ATP	O2'-C2'	-2.09	1.37	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ATP	O5'-C5'-C4'	15.30	161.08	108.99
3	B	704	ATP	O5'-C5'-C4'	14.36	157.90	108.99
3	B	704	ATP	O3A-PB-O1B	-8.62	84.78	110.70
3	A	701	ATP	O3A-PB-O1B	-6.89	89.99	110.70
3	A	701	ATP	O4'-C4'-C3'	6.73	118.51	105.15
3	B	704	ATP	O5'-PA-O1A	-6.66	82.53	108.94
3	A	701	ATP	O5'-PA-O1A	-6.65	82.56	108.94
3	A	701	ATP	C5'-C4'-C3'	-6.25	92.70	115.21
3	B	704	ATP	C5'-C4'-C3'	-5.73	94.59	115.21
3	B	704	ATP	PA-O5'-C5'	4.91	149.46	121.35
3	A	701	ATP	O2B-PB-O3A	-4.78	94.35	107.27
3	B	704	ATP	O2B-PB-O3B	4.22	118.68	107.27
3	A	701	ATP	O2B-PB-O3B	3.83	117.62	107.27
3	B	704	ATP	O2A-PA-O3A	3.71	117.31	107.27
3	B	704	ATP	O2B-PB-O3A	-3.63	97.47	107.27
3	A	701	ATP	O3A-PA-O1A	3.62	121.59	110.70
3	A	701	ATP	O4'-C4'-C5'	3.34	120.04	109.33
3	B	704	ATP	O3'-C3'-C4'	3.30	120.57	111.08
3	B	704	ATP	C6-C5-C4	-2.73	113.45	117.18
3	A	701	ATP	O3B-PB-O1B	2.72	118.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ATP	O4'-C1'-N9	2.66	113.19	108.09
3	B	704	ATP	O3A-PA-O1A	2.63	118.61	110.70
3	A	701	ATP	O2A-PA-O1A	2.62	124.65	112.44
3	B	704	ATP	O3B-PB-O1B	2.57	118.44	110.70
3	A	701	ATP	C4'-O4'-C1'	-2.50	103.95	109.47
3	B	704	ATP	O2A-PA-O1A	2.49	124.02	112.44
3	A	701	ATP	PA-O5'-C5'	2.48	135.54	121.35
3	A	701	ATP	O2A-PA-O3A	2.36	113.66	107.27
3	B	704	ATP	C3'-C2'-C1'	2.27	105.75	101.46
3	A	701	ATP	O3'-C3'-C2'	2.24	119.01	111.82
3	A	701	ATP	N9-C8-N7	-2.20	110.82	113.94
3	B	704	ATP	C5-C4-N3	2.19	129.73	126.72
3	B	704	ATP	N6-C6-N1	2.19	123.25	118.38
3	B	704	ATP	O2G-PG-O1G	2.17	119.27	110.83
3	A	701	ATP	C6-C5-C4	-2.07	114.35	117.18
3	A	701	ATP	O2'-C2'-C1'	2.04	117.14	110.10
3	A	701	ATP	O2B-PB-O1B	2.01	121.81	112.44

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	704	ATP	C2'-C1'-N9-C4
3	B	704	ATP	C2'-C1'-N9-C8
3	B	704	ATP	C4'-C5'-O5'-PA
3	A	701	ATP	C3'-C4'-C5'-O5'
3	A	701	ATP	C2'-C1'-N9-C4
3	A	701	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	PA-O3A-PB-O1B
3	A	701	ATP	C2'-C1'-N9-C8
3	A	701	ATP	PG-O3B-PB-O2B
3	B	704	ATP	PG-O3B-PB-O2B

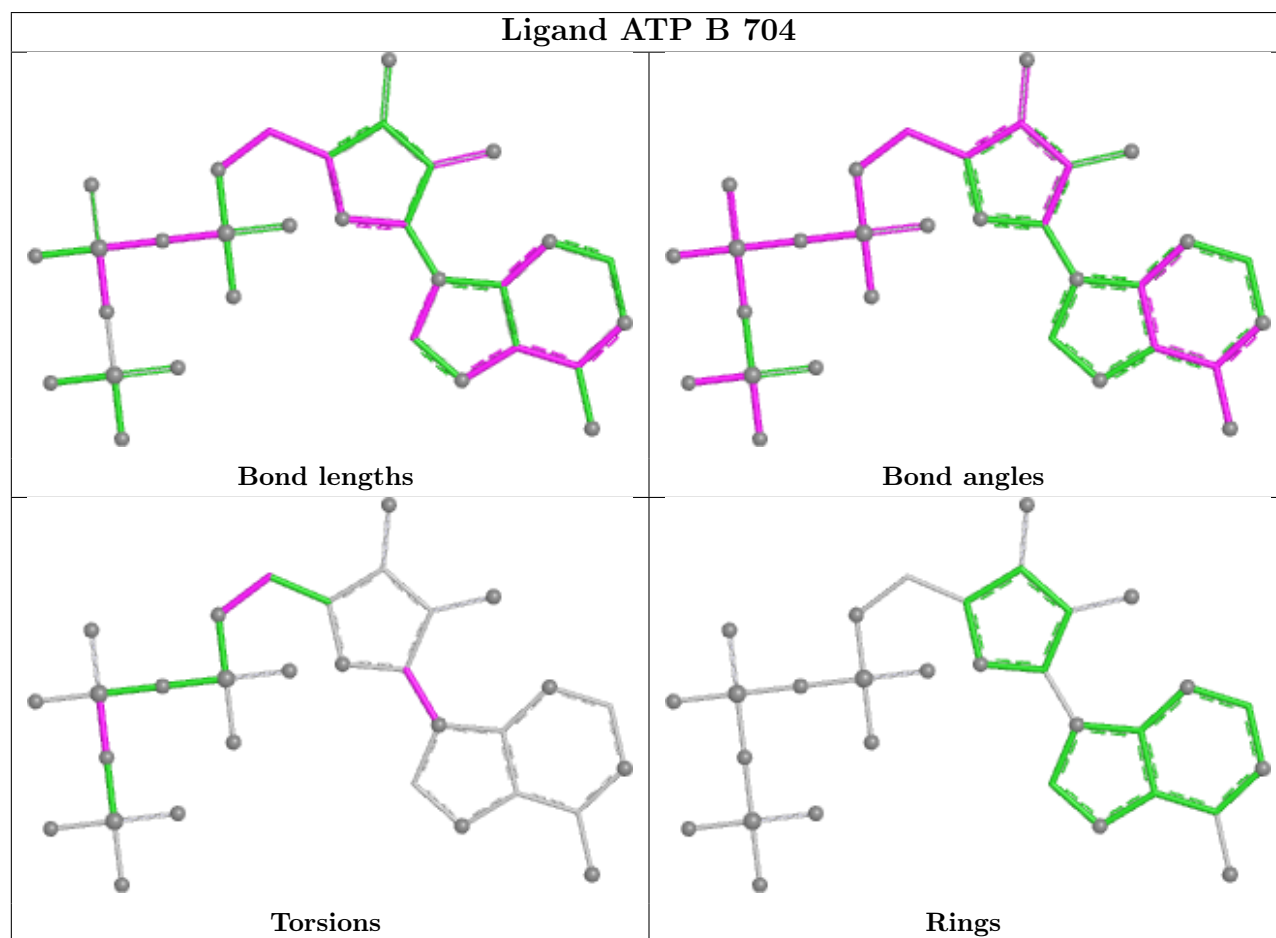
There are no ring outliers.

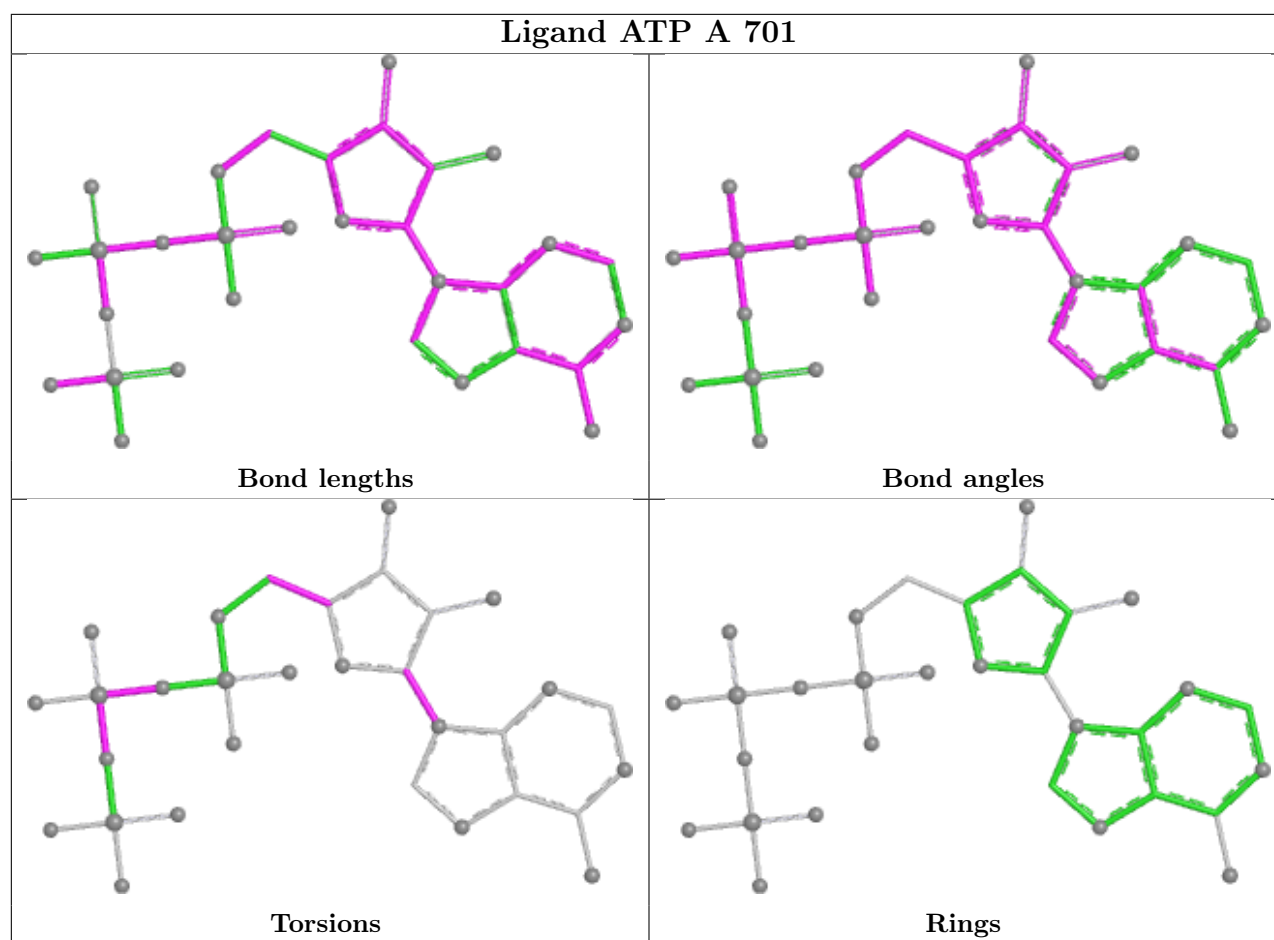
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	704	ATP	5	0
3	A	701	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	687/687 (100%)	0.74	111 (16%) 4 3	8, 29, 91, 136	0
1	B	687/687 (100%)	0.86	113 (16%) 4 3	8, 32, 92, 135	0
All	All	1374/1374 (100%)	0.80	224 (16%) 4 3	8, 30, 92, 136	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	ASN	9.3
1	A	405	ARG	7.5
1	B	412	ILE	7.4
1	A	238	GLU	7.3
1	A	411	ASN	7.2
1	B	241	ALA	7.0
1	B	404	ALA	6.7
1	B	414	TRP	6.5
1	A	412	ILE	6.3
1	B	405	ARG	6.2
1	A	241	ALA	6.1
1	B	239	MET	6.1
1	B	406	PHE	6.0
1	A	235	LEU	6.0
1	B	246	LEU	5.9
1	A	414	TRP	5.7
1	B	235	LEU	5.7
1	B	410	ALA	5.6
1	A	407	ASP	5.6
1	B	243	LEU	5.5
1	A	406	PHE	5.5
1	A	239	MET	5.4
1	A	404	ALA	5.2
1	B	413	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	374	TYR	5.1
1	A	246	LEU	5.1
1	A	70	ASN	5.1
1	A	254	ARG	5.0
1	B	377	ALA	4.8
1	B	188	GLU	4.7
1	B	69	SER	4.7
1	A	429	ALA	4.6
1	B	254	ARG	4.6
1	B	245	GLU	4.6
1	B	417	ARG	4.5
1	A	410	ALA	4.5
1	B	407	ASP	4.5
1	A	251	LEU	4.4
1	B	402	LEU	4.4
1	B	250	SER	4.3
1	A	413	HIS	4.3
1	A	237	HIS	4.3
1	B	415	ALA	4.2
1	A	375	ARG	4.2
1	A	402	LEU	4.2
1	A	236	VAL	4.2
1	A	240	GLU	4.1
1	A	245	GLU	4.1
1	A	243	LEU	4.1
1	A	403	GLN	4.0
1	A	415	ALA	4.0
1	B	236	VAL	4.0
1	A	188	GLU	4.0
1	A	255	LEU	4.0
1	B	240	GLU	3.9
1	B	403	GLN	3.9
1	B	247	MET	3.9
1	B	70	ASN	3.9
1	A	252	LYS	3.9
1	B	249	SER	3.9
1	A	69	SER	3.8
1	B	374	TYR	3.7
1	B	620	TYR	3.7
1	A	408	GLU	3.7
1	A	285	TYR	3.7
1	B	190	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	244	MET	3.7
1	B	285	TYR	3.6
1	A	2	GLY	3.6
1	B	233	TYR	3.6
1	B	71	SER	3.6
1	A	193	ARG	3.6
1	A	377	ALA	3.5
1	A	249	SER	3.5
1	B	4	GLU	3.5
1	A	191	ARG	3.4
1	B	520	ARG	3.4
1	A	71	SER	3.4
1	B	248	SER	3.4
1	B	251	LEU	3.4
1	A	73	SER	3.4
1	B	242	SER	3.4
1	A	688	GLU	3.4
1	A	256	THR	3.4
1	A	250	SER	3.4
1	B	256	THR	3.3
1	B	408	GLU	3.3
1	A	61	ILE	3.3
1	A	416	LYS	3.3
1	B	189	ALA	3.3
1	A	244	MET	3.2
1	B	419	THR	3.2
1	B	3	GLN	3.2
1	A	242	SER	3.2
1	B	688	GLU	3.2
1	B	291	GLY	3.2
1	A	248	SER	3.2
1	A	65	GLU	3.2
1	A	247	MET	3.2
1	A	149	PHE	3.1
1	B	230	ASP	3.1
1	B	238	GLU	3.1
1	B	259	PRO	3.1
1	B	255	LEU	3.1
1	A	417	ARG	3.1
1	A	258	GLU	3.1
1	B	252	LYS	3.1
1	B	378	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	231	ALA	3.0
1	A	189	ALA	3.0
1	B	234	ASP	3.0
1	A	282	ILE	3.0
1	B	5	LYS	3.0
1	B	237	HIS	2.9
1	B	257	ALA	2.9
1	B	193	ARG	2.9
1	A	376	VAL	2.9
1	A	59	ARG	2.9
1	B	409	GLU	2.9
1	A	280	LEU	2.9
1	B	432	LEU	2.9
1	A	509	ASN	2.9
1	B	575	GLY	2.9
1	A	62	ILE	2.9
1	B	376	VAL	2.8
1	A	186	PRO	2.8
1	B	150	LEU	2.8
1	B	64	SER	2.8
1	B	72	HIS	2.8
1	B	429	ALA	2.8
1	A	418	LEU	2.8
1	B	416	LYS	2.8
1	B	63	ILE	2.8
1	A	310	ASN	2.8
1	A	378	LYS	2.8
1	A	253	GLN	2.8
1	A	233	TYR	2.7
1	B	266	ARG	2.7
1	B	61	ILE	2.7
1	B	667	ASN	2.7
1	B	418	LEU	2.7
1	A	3	GLN	2.7
1	B	261	ARG	2.7
1	A	409	GLU	2.7
1	A	68	GLY	2.6
1	A	192	ARG	2.6
1	B	260	VAL	2.6
1	B	574	GLU	2.6
1	A	257	ALA	2.6
1	A	419	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	148	GLN	2.6
1	B	430	PRO	2.6
1	B	2	GLY	2.6
1	B	129	GLN	2.6
1	A	228	THR	2.6
1	B	104	ARG	2.6
1	B	509	ASN	2.6
1	A	187	PRO	2.5
1	B	182	PHE	2.5
1	B	57	LEU	2.5
1	B	427	PHE	2.5
1	A	668	ARG	2.5
1	A	124	ARG	2.5
1	B	181	ARG	2.5
1	A	281	THR	2.5
1	A	428	SER	2.5
1	A	314	LYS	2.4
1	A	74	ARG	2.4
1	A	259	PRO	2.4
1	A	291	GLY	2.4
1	B	62	ILE	2.4
1	A	427	PHE	2.4
1	A	144	THR	2.4
1	A	232	GLU	2.4
1	B	73	SER	2.4
1	A	307	GLY	2.4
1	B	192	ARG	2.4
1	A	151	LYS	2.4
1	A	373	ILE	2.4
1	A	190	PRO	2.3
1	A	666	GLY	2.3
1	B	58	LYS	2.3
1	B	253	GLN	2.3
1	B	686	GLN	2.3
1	A	667	ASN	2.3
1	A	262	PHE	2.3
1	A	260	VAL	2.3
1	A	118	ASN	2.3
1	B	121	ASN	2.3
1	A	148	GLN	2.3
1	A	145	ASP	2.3
1	A	278	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	129	GLN	2.2
1	B	299	ASP	2.2
1	B	65	GLU	2.2
1	A	147	VAL	2.2
1	B	529	LEU	2.2
1	A	165	ASP	2.2
1	A	261	ARG	2.2
1	B	186	PRO	2.2
1	A	5	LYS	2.2
1	B	314	LYS	2.2
1	A	130	TYR	2.1
1	A	229	ARG	2.1
1	B	229	ARG	2.1
1	B	144	THR	2.1
1	B	373	ILE	2.1
1	B	59	ARG	2.1
1	B	176	SER	2.1
1	B	89	GLN	2.1
1	B	97	GLU	2.1
1	B	287	SER	2.1
1	A	227	MET	2.1
1	A	601	GLY	2.1
1	B	83	ARG	2.1
1	B	191	ARG	2.1
1	B	232	GLU	2.1
1	A	63	ILE	2.1
1	A	234	ASP	2.1
1	B	375	ARG	2.0
1	B	431	GLY	2.0
1	A	283	SER	2.0
1	A	60	ARG	2.0
1	B	315	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

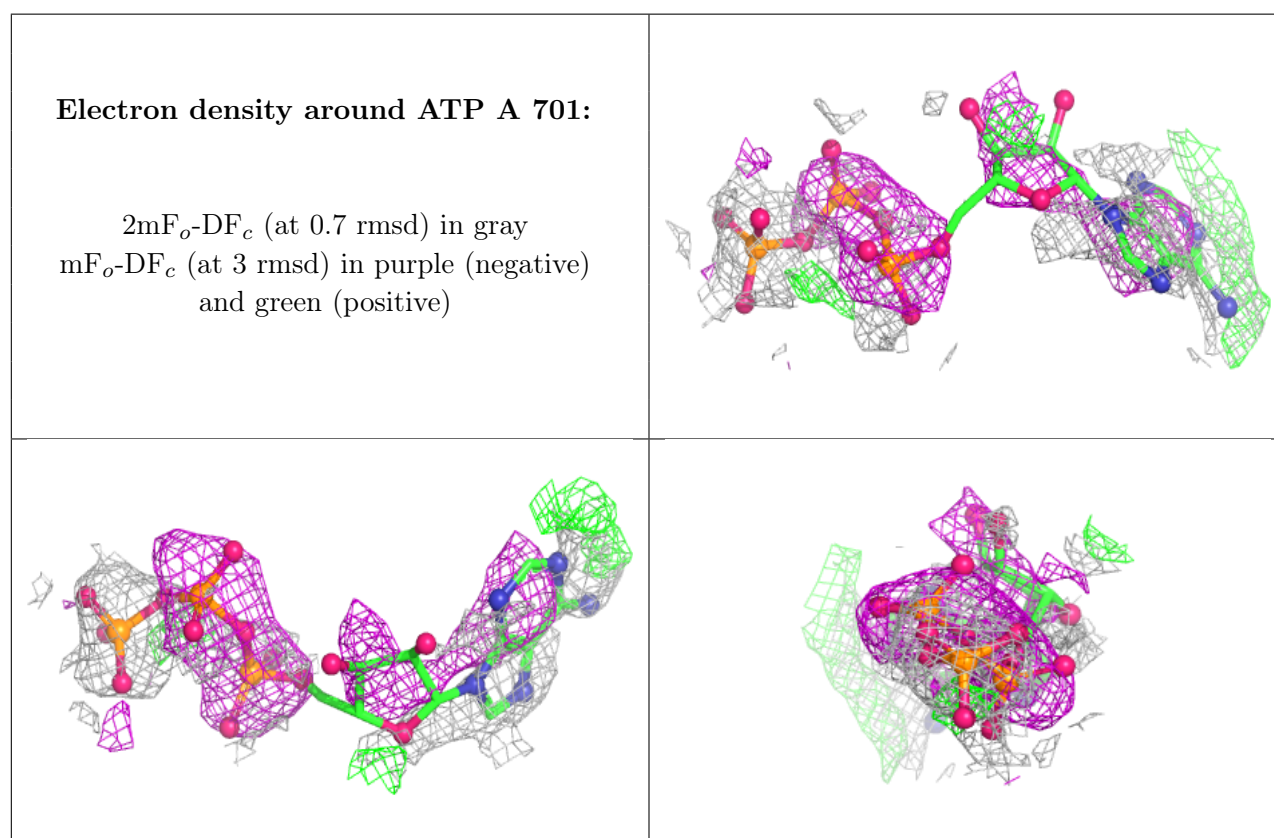
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

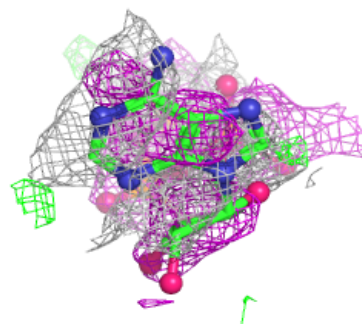
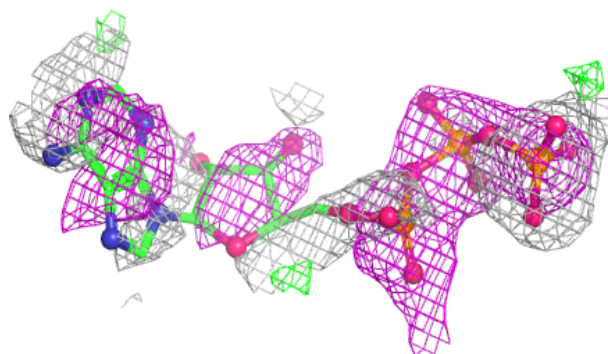
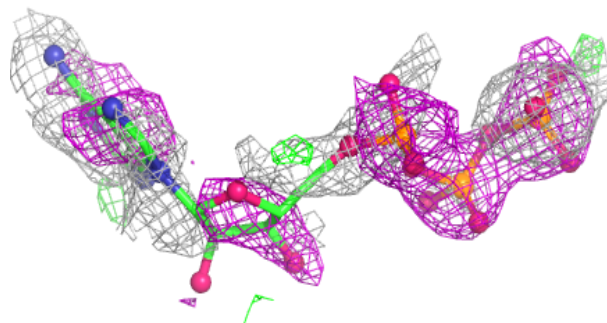
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	703	1/1	0.11	0.40	79,79,79,79	0
3	ATP	A	701	31/31	0.33	0.27	59,67,71,71	0
3	ATP	B	704	31/31	0.49	0.24	61,65,67,68	0
2	MG	B	705	1/1	0.57	0.51	68,68,68,68	0
2	MG	A	702	1/1	0.63	0.30	58,58,58,58	0
2	MG	B	706	1/1	0.72	0.59	88,88,88,88	0

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 704:

$2mF_o-DF_c$ (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.