



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:05 PM EDT

PDB ID : 3ETJ / pdb_00003etj
Title : Crystal structure E. coli Purk in complex with Mg, ADP, and Pi
Authors : Holden, H.M.; Thoden, J.B.
Deposited on : 2008-10-08
Resolution : 1.60 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

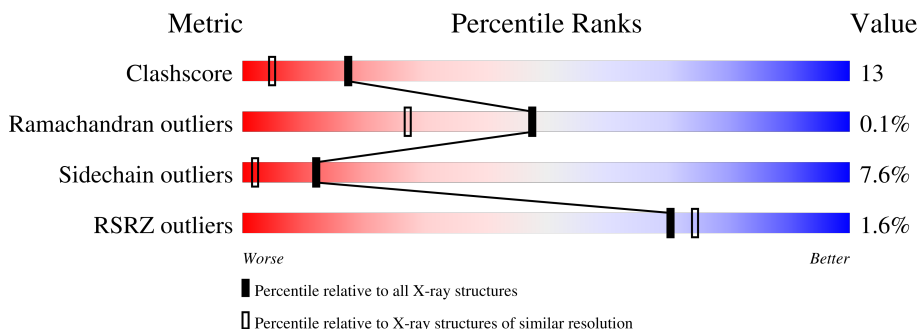
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	355	% 66% 28% • •
1	B	355	3% 67% 25% 6% • •

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
4	PI	B	403	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6305 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.

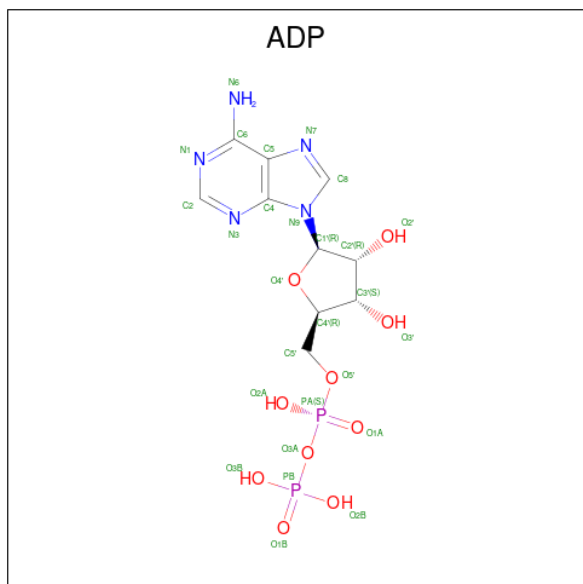
- Molecule 1 is a protein called Phosphoribosylaminoimidazole carboxylase ATPase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	2	0
			2793	1777	495	510	11			
1	B	351	Total	C	N	O	S	0	3	0
			2762	1758	491	502	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	GLU	engineered mutation	UNP P09029
A	205	ARG	GLN	engineered mutation	UNP P09029
B	61	GLN	GLU	engineered mutation	UNP P09029
B	205	ARG	GLN	engineered mutation	UNP P09029

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

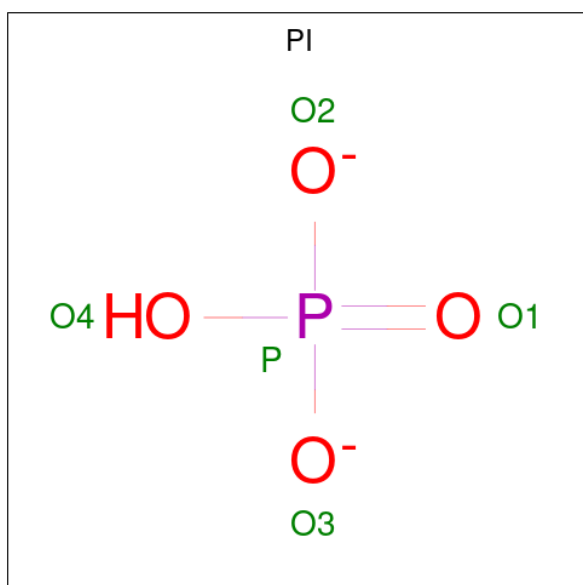


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is HYDROGENPHOSPHATE ION (CCD ID: PI) (formula: HO_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

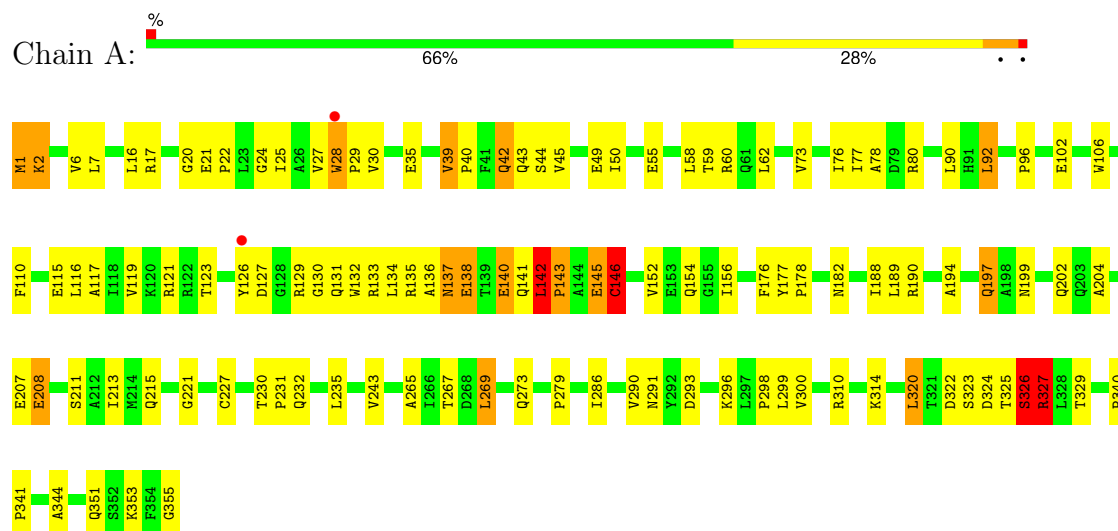
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	384	Total 384	O 384	0	0
6	B	297	Total 297	O 297	0	0

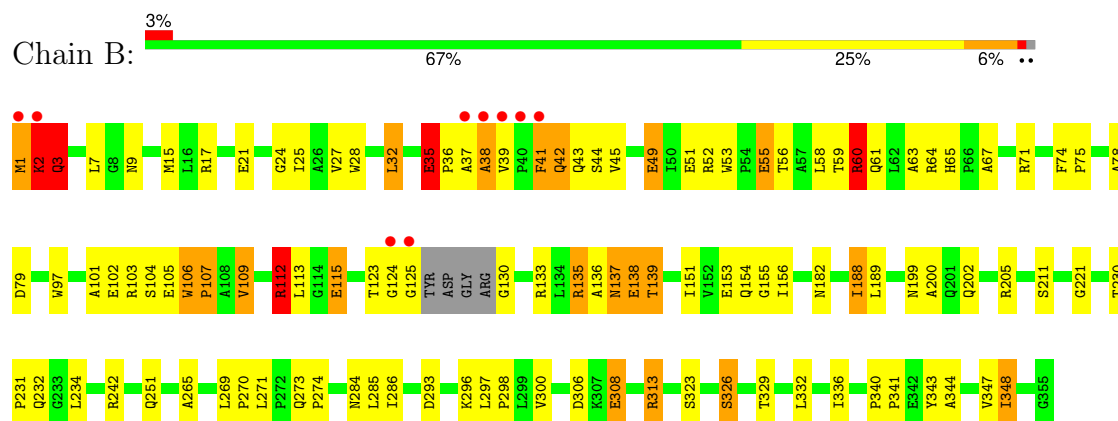
3 Residue-property plots

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

• Molecule 1: Phosphoribosylaminoimidazole carboxylase ATPase subunit



• Molecule 1: Phosphoribosylaminoimidazole carboxylase ATPase subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.80Å 70.50Å 88.70Å 90.00° 124.30° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-1.60) 93.5 (30.00-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 1.60Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.158 , 0.215 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 89.9	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	0.97	EDS
Total number of atoms	6305	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% 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, CL, PI, ADP

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	0.99	2/2871 (0.1%)	1.75	58/3912 (1.5%)
1	B	0.93	0/2842	1.77	59/3871 (1.5%)
All	All	0.96	2/5713 (0.0%)	1.76	117/7783 (1.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	VAL	CA-CB	5.75	1.61	1.54
1	A	290	VAL	CA-CB	5.04	1.59	1.54

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	VAL	N-CA-C	-11.88	91.01	108.71
1	B	106	TRP	N-CA-C	10.60	128.19	113.45
1	B	109	VAL	N-CA-C	-10.41	100.74	110.53
1	A	142	LEU	N-CA-C	9.70	123.78	109.42
1	B	139	THR	N-CA-C	8.89	123.90	112.34
1	B	41	PHE	CB-CA-C	8.33	123.95	110.88
1	A	327	ARG	CB-CA-C	-8.07	97.39	110.79
1	B	105	GLU	N-CA-C	7.79	121.88	112.38
1	A	62	LEU	N-CA-C	7.62	119.38	111.14
1	B	200	ALA	N-CA-C	7.58	120.62	111.82
1	A	28	TRP	CB-CA-C	-7.57	102.61	110.33
1	B	59	THR	N-CA-C	7.54	120.38	111.71
1	B	112	ARG	N-CA-C	7.54	120.96	111.69
1	A	45	VAL	N-CA-C	-7.35	97.99	108.58
1	A	197	GLN	CB-CA-C	-7.24	98.14	110.16
1	A	106	TRP	CA-C-O	7.15	125.16	118.44
1	B	101	ALA	N-CA-C	7.06	120.37	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	SER	N-CA-C	-7.05	103.35	112.23
1	B	53	TRP	N-CA-C	-7.04	101.89	108.22
1	B	348	ILE	CB-CG1-CD1	-6.99	99.12	113.80
1	B	211	SER	CB-CA-C	-6.98	99.20	110.79
1	B	60	ARG	N-CA-C	-6.92	103.73	111.28
1	A	35	GLU	N-CA-C	-6.91	101.08	109.72
1	B	138	GLU	N-CA-C	6.89	121.70	113.16
1	B	78	ALA	CA-C-N	-6.87	113.91	122.84
1	B	78	ALA	C-N-CA	-6.87	113.91	122.84
1	A	115	GLU	N-CA-C	6.76	119.49	111.71
1	A	207	GLU	CA-C-N	-6.76	110.69	120.29
1	A	207	GLU	C-N-CA	-6.76	110.69	120.29
1	A	62	LEU	CB-CA-C	-6.72	100.29	110.90
1	A	16	LEU	N-CA-C	-6.65	104.11	111.36
1	A	310	ARG	CB-CA-C	6.64	120.27	109.97
1	B	293	ASP	N-CA-C	-6.61	104.10	111.71
1	A	115	GLU	CA-C-N	-6.55	113.11	122.94
1	A	115	GLU	C-N-CA	-6.55	113.11	122.94
1	B	155	GLY	N-CA-C	-6.48	100.86	110.97
1	A	326	SER	N-CA-C	-6.42	104.38	111.82
1	A	320	LEU	CB-CG-CD2	-6.36	91.62	110.70
1	A	76	ILE	N-CA-C	6.24	116.99	110.62
1	B	139	THR	OG1-CB-CG2	6.23	121.76	109.30
1	B	344	ALA	N-CA-C	6.23	118.58	111.11
1	A	20	GLY	N-CA-C	6.21	121.69	113.37
1	B	341	PRO	N-CA-C	6.20	122.02	113.65
1	A	135	ARG	CB-CA-C	6.18	120.00	109.80
1	B	135[A]	ARG	N-CA-C	-6.16	100.11	109.85
1	B	135[B]	ARG	N-CA-C	-6.16	100.11	109.85
1	B	41	PHE	N-CA-C	6.15	117.65	111.07
1	A	102	GLU	N-CA-CB	-6.14	102.03	111.56
1	A	134	LEU	N-CA-C	6.14	119.40	109.40
1	B	56	THR	N-CA-C	-6.10	100.52	109.18
1	B	151	ILE	N-CA-C	-6.06	100.69	109.29
1	B	2	LYS	N-CA-CB	-6.05	101.87	110.46
1	A	102	GLU	CB-CA-C	-6.04	99.38	110.62
1	B	199	ASN	N-CA-C	-6.03	101.26	110.30
1	A	199	ASN	N-CA-C	-6.00	101.03	109.96
1	B	51	GLU	N-CA-C	5.98	120.74	112.90
1	B	35	GLU	N-CA-C	-5.98	102.12	109.65
1	B	97	TRP	N-CA-CB	-5.95	101.84	111.24
1	A	59	THR	N-CA-CB	5.89	118.79	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LYS	N-CA-C	-5.79	106.18	113.18
1	A	211	SER	N-CA-C	-5.77	105.07	111.36
1	A	202	GLN	N-CA-CB	-5.71	101.72	110.12
1	A	299	LEU	N-CA-C	-5.71	106.32	113.28
1	B	348	ILE	CA-CB-CG2	5.68	120.16	110.50
1	A	138	GLU	N-CA-C	5.68	120.21	112.88
1	B	49	GLU	N-CA-C	-5.66	105.58	112.88
1	A	92	LEU	CA-C-O	5.65	122.96	119.29
1	B	348	ILE	N-CA-CB	-5.63	102.14	110.58
1	A	135	ARG	N-CA-C	-5.60	101.74	110.42
1	A	351	GLN	CB-CA-C	-5.57	101.55	110.79
1	A	178	PRO	CB-CA-C	-5.56	103.94	111.12
1	A	298	PRO	N-CA-C	5.52	121.02	113.84
1	A	213	ILE	N-CA-CB	-5.51	104.10	110.55
1	A	133	ARG	N-CA-CB	5.46	119.28	110.65
1	A	39	VAL	CA-C-N	5.40	126.59	119.84
1	A	39	VAL	C-N-CA	5.40	126.59	119.84
1	B	265	ALA	N-CA-C	5.36	116.81	111.07
1	B	3	GLN	CA-CB-CG	-5.33	103.44	114.10
1	A	300	VAL	N-CA-C	5.33	116.43	108.54
1	B	139	THR	N-CA-CB	-5.33	100.59	110.18
1	A	353	LYS	CA-C-N	-5.32	114.64	122.83
1	A	353	LYS	C-N-CA	-5.32	114.64	122.83
1	B	115	GLU	N-CA-C	5.25	117.00	111.28
1	B	21	GLU	CB-CG-CD	-5.24	103.69	112.60
1	A	96	PRO	N-CA-C	-5.23	102.88	111.15
1	B	251	GLN	CA-C-N	-5.22	114.03	122.23
1	B	251	GLN	C-N-CA	-5.22	114.03	122.23
1	B	300	VAL	N-CA-C	5.20	115.71	108.84
1	A	80	ARG	N-CA-C	5.20	118.40	111.75
1	B	221	GLY	CA-C-O	-5.18	117.25	121.76
1	B	297	LEU	N-CA-CB	-5.18	103.59	110.17
1	B	32	LEU	N-CA-C	5.17	118.69	112.38
1	A	121	ARG	CB-CA-C	-5.17	100.37	109.62
1	A	60	ARG	CG-CD-NE	-5.16	100.64	112.00
1	A	146	CYS	CB-CA-C	-5.15	102.23	110.79
1	B	340	PRO	CB-CA-C	-5.13	104.66	110.92
1	B	298	PRO	N-CA-C	5.13	120.57	113.65
1	A	177	TYR	N-CA-C	-5.11	103.51	110.36
1	A	344	ALA	N-CA-C	5.11	117.24	111.11
1	B	285	LEU	N-CA-C	-5.10	100.20	108.52
1	A	44	SER	CB-CA-C	-5.09	99.32	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	PRO	N-CA-C	-5.09	104.49	110.70
1	B	156	ILE	CA-C-N	-5.09	114.52	122.05
1	B	156	ILE	C-N-CA	-5.09	114.52	122.05
1	A	2	LYS	CB-CA-C	5.09	118.13	109.53
1	B	15	MET	CA-CB-CG	-5.08	103.94	114.10
1	B	136	ALA	N-CA-C	5.06	118.23	111.75
1	B	293	ASP	CA-C-N	-5.04	113.02	120.28
1	B	293	ASP	C-N-CA	-5.04	113.02	120.28
1	A	29	PRO	N-CA-C	-5.04	102.59	110.50
1	A	55	GLU	CB-CA-C	-5.03	101.55	109.80
1	A	208	GLU	N-CA-CB	-5.03	102.71	110.16
1	A	227	CYS	N-CA-CB	-5.02	103.44	111.43
1	A	25	ILE	CA-C-O	5.02	125.90	120.53
1	B	313	ARG	CB-CG-CD	-5.02	99.76	111.30
1	B	271	LEU	CB-CA-C	5.01	117.78	111.21
1	A	130	GLY	N-CA-C	-5.00	106.25	114.76

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	2793	0	2769	69	1
1	B	2762	0	2747	69	1
2	A	27	0	12	1	0
2	B	27	0	12	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	1	0	0	1	0
6	A	384	0	0	3	2
6	B	297	0	0	6	2
All	All	6305	0	5540	140	4

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 13.

All (140) 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:324:ASP:HB3	1:A:327:ARG:HG3	1.21	1.13
1:B:1:MET:HG2	1:B:2:LYS:H	1.11	1.11
1:B:202:GLN:HA	1:B:205:ARG:HH12	1.07	1.11
1:B:135[A]:ARG:HH11	1:B:135[A]:ARG:HG2	1.16	1.05
1:B:202:GLN:HA	1:B:205:ARG:NH1	1.73	1.03
1:B:102:GLU:HG3	1:B:104:SER:HB2	1.51	0.92
1:B:35:GLU:H	1:B:35:GLU:CD	1.76	0.89
1:A:230:THR:HB	1:A:231:PRO:HD2	1.56	0.87
1:B:1:MET:HG2	1:B:2:LYS:N	1.89	0.86
1:B:135[A]:ARG:HG2	1:B:135[A]:ARG:NH1	1.88	0.85
1:B:36:PRO:HG3	1:B:58:LEU:HA	1.61	0.81
1:A:2:LYS:HE3	1:A:267:THR:HB	1.64	0.79
1:A:126:TYR:OH	1:A:129:ARG:NH1	2.16	0.79
1:B:308:GLU:O	1:B:313:ARG:NH1	2.17	0.78
1:B:112:ARG:HG2	1:B:112:ARG:HH11	1.50	0.77
1:B:1:MET:CG	1:B:2:LYS:H	1.90	0.76
1:B:112:ARG:HH11	1:B:112:ARG:CG	1.98	0.76
1:A:143:PRO:HB3	1:A:145:GLU:OE1	1.87	0.74
1:A:2:LYS:HE2	1:A:269:LEU:HD11	1.71	0.72
1:A:324:ASP:CG	1:A:326:SER:HG	1.99	0.70
1:B:113:LEU:O	1:B:154:GLN:HG3	1.92	0.70
1:A:42:GLN:H	1:A:42:GLN:CD	2.00	0.68
1:A:230:THR:HB	1:A:231:PRO:CD	2.22	0.68
1:A:1:MET:HG2	1:A:2:LYS:O	1.94	0.67
1:A:7:LEU:CD2	1:A:50:ILE:HD11	2.23	0.67
1:B:242:ARG:HB3	6:B:459:HOH:O	1.95	0.66
1:B:326[A]:SER:OG	6:B:653:HOH:O	2.12	0.66
1:A:204:ALA:HB3	6:A:757:HOH:O	1.95	0.65
1:B:188:ILE:C	1:B:188:ILE:HD13	2.21	0.65
1:A:230:THR:CB	1:A:231:PRO:HD2	2.27	0.65
1:A:143:PRO:O	1:A:146:CYS:HB2	1.97	0.64
1:B:55:GLU:HG3	6:B:680:HOH:O	1.97	0.64
1:A:73:VAL:HG12	1:A:77:ILE:HD12	1.78	0.64
1:A:73:VAL:CG1	1:A:77:ILE:HD11	2.27	0.64
1:A:110:PHE:CE1	1:A:136:ALA:HA	2.33	0.64
1:A:324:ASP:CB	1:A:327:ARG:HG3	2.12	0.63
1:A:73:VAL:HG12	1:A:77:ILE:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:GLN:NE2	6:B:521:HOH:O	2.32	0.62
1:B:39:VAL:HG12	1:B:41:PHE:HB3	1.80	0.61
1:B:242:ARG:HD3	6:B:459:HOH:O	1.99	0.61
1:B:1:MET:CG	1:B:2:LYS:N	2.55	0.61
1:A:116:LEU:H	1:A:116:LEU:HD23	1.66	0.60
1:B:1:MET:HG2	1:B:2:LYS:HG2	1.83	0.60
1:A:7:LEU:HD23	1:A:50:ILE:HD11	1.85	0.59
1:A:137:ASN:HD22	1:A:138:GLU:HG3	1.68	0.59
1:A:126:TYR:CD2	1:A:126:TYR:N	2.71	0.58
1:A:324:ASP:O	1:A:327:ARG:HB2	2.04	0.58
1:A:322:ASP:CG	1:A:327:ARG:HD2	2.29	0.58
1:A:73:VAL:CG1	1:A:77:ILE:CD1	2.82	0.58
1:A:17:ARG:HA	1:A:27:VAL:HB	1.85	0.57
1:A:324:ASP:HB3	1:A:327:ARG:CG	2.14	0.57
1:A:116:LEU:HD23	1:A:116:LEU:N	2.18	0.57
1:B:3:GLN:CD	1:B:28:TRP:HE1	2.11	0.57
1:B:65:HIS:CE1	1:B:67:ALA:HB3	2.41	0.56
1:A:7:LEU:HD21	1:A:50:ILE:HD11	1.86	0.56
1:A:324:ASP:OD1	1:A:327:ARG:N	2.36	0.56
1:A:1:MET:HG2	1:A:2:LYS:N	2.18	0.56
1:A:230:THR:CB	1:A:231:PRO:CD	2.82	0.56
1:B:188:ILE:HD13	1:B:189:LEU:O	2.05	0.56
1:B:202:GLN:CA	1:B:205:ARG:HH12	1.99	0.55
1:B:17:ARG:HA	1:B:27:VAL:HB	1.89	0.55
1:B:135[A]:ARG:NH1	1:B:135[A]:ARG:CG	2.61	0.55
1:B:137:ASN:OD1	1:B:137:ASN:N	2.38	0.55
1:A:78:ALA:O	1:A:123:THR:HG22	2.07	0.54
1:B:55:GLU:OE2	1:B:60:ARG:HG3	2.08	0.53
1:A:2:LYS:HE2	1:A:269:LEU:CD1	2.37	0.53
1:B:202:GLN:CG	1:B:205:ARG:HH12	2.22	0.52
1:A:141:GLN:O	1:A:143:PRO:HD3	2.09	0.52
1:B:1:MET:HE2	1:B:24:GLY:O	2.10	0.52
1:B:37:ALA:C	1:B:39:VAL:H	2.18	0.52
1:A:30:VAL:HG11	1:A:58:LEU:HD21	1.93	0.51
1:B:35:GLU:OE2	1:B:38:ALA:HB3	2.11	0.51
1:A:208:GLU:HB2	6:A:632:HOH:O	2.10	0.50
1:B:124:GLY:O	1:B:125:GLY:O	2.28	0.50
1:B:36:PRO:HB3	1:B:61:GLN:HG3	1.94	0.50
1:B:205:ARG:HD2	1:B:234:LEU:HB2	1.93	0.50
1:B:1:MET:HG2	1:B:2:LYS:CG	2.42	0.49
1:B:188:ILE:HD13	1:B:189:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:HB3	1:A:22:PRO:HD3	1.94	0.49
1:B:273:GLN:NE2	1:B:274:PRO:HD2	2.28	0.49
1:A:127:ASP:OD1	1:A:314:LYS:NZ	2.34	0.48
1:B:42:GLN:H	1:B:42:GLN:CD	2.22	0.48
2:B:400:ADP:O2B	4:B:403:PI:O4	2.32	0.48
1:A:1:MET:HB2	6:A:532:HOH:O	2.14	0.48
1:A:90:LEU:HB2	1:A:92:LEU:HG	1.96	0.48
1:B:230:THR:HB	1:B:231:PRO:HD2	1.95	0.47
1:A:325:THR:O	1:A:329:THR:HG23	2.13	0.47
1:A:39:VAL:HA	1:A:40:PRO:HD3	1.75	0.47
1:A:42:GLN:H	1:A:42:GLN:NE2	2.12	0.47
1:B:55:GLU:OE1	6:B:681:HOH:O	2.20	0.47
1:A:28:TRP:CD1	1:A:28:TRP:N	2.83	0.46
1:A:154:GLN:HE21	1:A:156:ILE:HD13	1.80	0.46
1:B:39:VAL:O	1:B:41:PHE:N	2.42	0.46
1:A:142:LEU:HG	1:A:146:CYS:SG	2.56	0.46
1:A:73:VAL:HG13	1:A:77:ILE:HD11	1.97	0.46
1:B:182:ASN:HB3	1:B:189:LEU:CD1	2.46	0.45
1:B:74:PHE:HB2	1:B:75:PRO:HD3	1.98	0.45
1:A:132:TRP:N	1:A:132:TRP:CE3	2.85	0.45
1:A:176:PHE:O	1:A:273:GLN:NE2	2.37	0.45
1:A:117:ALA:HB1	1:A:152:VAL:HG21	1.99	0.44
1:A:119:VAL:O	1:A:131:GLN:HA	2.16	0.44
1:A:127:ASP:HB3	1:A:188:ILE:HD12	1.99	0.44
1:B:286:ILE:HA	1:B:313:ARG:O	2.17	0.44
1:A:142:LEU:HA	1:A:143:PRO:HD2	1.93	0.44
1:B:2:LYS:HB3	1:B:25:ILE:HG12	2.00	0.44
1:B:112:ARG:HG2	1:B:112:ARG:NH1	2.26	0.44
1:B:231:PRO:HB2	1:B:232:GLN:NE2	2.32	0.44
1:A:291:ASN:OD1	1:A:293:ASP:HB2	2.18	0.43
1:B:3:GLN:HG2	1:B:44:SER:OG	2.18	0.43
1:B:329:THR:HA	1:B:332:LEU:HD12	2.00	0.43
1:A:221:GLY:HA2	1:A:265:ALA:HB3	1.99	0.43
1:B:188:ILE:CD1	1:B:189:LEU:O	2.67	0.43
1:B:205:ARG:NH1	1:B:205:ARG:HB3	2.34	0.43
1:B:269:LEU:HB3	1:B:270:PRO:CD	2.49	0.42
1:A:243:VAL:HG22	5:A:404:CL:CL	2.56	0.42
1:B:7:LEU:HD11	1:B:32:LEU:HD23	2.01	0.42
1:A:194:ALA:O	1:A:279:PRO:HA	2.20	0.41
1:A:1:MET:HG3	1:A:24:GLY:O	2.20	0.41
1:A:42:GLN:CD	1:A:42:GLN:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLN:HG3	1:B:205:ARG:HH12	1.86	0.41
1:B:348:ILE:HG21	1:B:348:ILE:HD13	1.60	0.41
1:B:63:ALA:O	1:B:64:ARG:HB2	2.21	0.41
1:B:284:ASN:O	1:B:343:TYR:HE2	2.03	0.41
1:B:2:LYS:HB2	1:B:25:ILE:HA	2.03	0.41
1:A:117:ALA:HB1	1:A:152:VAL:CG2	2.51	0.41
2:A:400:ADP:O2B	4:A:403:PI:O4	2.38	0.41
1:B:39:VAL:HG21	1:B:58:LEU:HD13	2.03	0.41
1:B:125:GLY:C	1:B:130:GLY:HA3	2.45	0.41
1:B:205:ARG:HB3	1:B:205:ARG:HH11	1.85	0.41
1:B:336:ILE:HG13	1:B:347:VAL:HG11	2.02	0.41
1:B:79:ASP:HA	1:B:123:THR:HG22	2.03	0.41
1:A:40:PRO:HA	1:A:42:GLN:HE22	1.86	0.40
1:A:182:ASN:HB3	1:A:189:LEU:HD13	2.02	0.40
1:B:106:TRP:HB2	1:B:107:PRO:HD3	2.03	0.40
1:B:308:GLU:N	1:B:313:ARG:HH12	2.19	0.40
1:A:324:ASP:OD1	1:A:326:SER:OG	2.15	0.40
1:A:340:PRO:HA	1:A:341:PRO:HD3	1.90	0.40
1:A:190:ARG:CZ	1:A:286:ILE:HD12	2.51	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:NE2	6:B:681:HOH:O[3_445]	2.15	0.05
1:B:135[A]:ARG:NH1	6:A:698:HOH:O[4_546]	2.16	0.04
6:B:646:HOH:O	6:B:646:HOH:O[2_657]	2.17	0.03
6:A:753:HOH:O	6:A:753:HOH:O[2_557]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	355/355 (100%)	348 (98%)	7 (2%)	0	100	100
1	B	350/355 (99%)	343 (98%)	6 (2%)	1 (0%)	36	20
All	All	705/710 (99%)	691 (98%)	13 (2%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	38	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	298/296 (101%)	279 (94%)	19 (6%)	16	3
1	B	296/296 (100%)	268 (90%)	28 (10%)	8	1
All	All	594/592 (100%)	547 (92%)	47 (8%)	12	2

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	42	GLN
1	A	43	GLN
1	A	49	GLU
1	A	137	ASN
1	A	140[A]	GLU
1	A	140[B]	GLU
1	A	142	LEU
1	A	143	PRO
1	A	145	GLU
1	A	146	CYS
1	A	197	GLN
1	A	232	GLN
1	A	235	LEU
1	A	269	LEU

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Mol	Chain	Res	Type
1	A	320	LEU
1	A	323	SER
1	A	326	SER
1	A	327	ARG
1	B	1	MET
1	B	2	LYS
1	B	3	GLN
1	B	9	ASN
1	B	35	GLU
1	B	42	GLN
1	B	43	GLN
1	B	49	GLU
1	B	52	ARG
1	B	55	GLU
1	B	60	ARG
1	B	71	ARG
1	B	103	ARG
1	B	107	PRO
1	B	109	VAL
1	B	112	ARG
1	B	115	GLU
1	B	133	ARG
1	B	137	ASN
1	B	138	GLU
1	B	139	THR
1	B	153	GLU
1	B	188	ILE
1	B	296	LYS
1	B	306	ASP
1	B	308	GLU
1	B	326[A]	SER
1	B	326[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	42	GLN
1	A	43	GLN
1	A	137	ASN
1	A	141	GLN
1	A	154	GLN

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Mol	Chain	Res	Type
1	A	232	GLN
1	A	278	ASN
1	B	61	GLN
1	B	141	GLN
1	B	232	GLN
1	B	273	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	B	400	3	28,29,29	1.13	4 (14%)	43,45,45	1.86	14 (32%)
4	PI	B	403	3	4,4,4	2.45	4 (100%)	6,6,6	1.89	2 (33%)
4	PI	A	403	3	4,4,4	1.80	2 (50%)	6,6,6	0.74	0
2	ADP	A	400	3	28,29,29	1.16	3 (10%)	43,45,45	1.51	8 (18%)

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	B	400	3	-	2/16/32/32	0/3/3/3
2	ADP	A	400	3	-	2/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	ADP	C6-N6	-3.44	1.25	1.34
2	B	400	ADP	C6-N6	-3.09	1.26	1.34
4	B	403	PI	P-O4	-2.57	1.47	1.54
2	A	400	ADP	C2-N1	2.56	1.38	1.33
4	B	403	PI	P-O3	-2.51	1.47	1.54
4	B	403	PI	P-O2	-2.47	1.47	1.54
4	A	403	PI	P-O3	-2.36	1.47	1.54
4	B	403	PI	P-O1	-2.25	1.45	1.50
2	B	400	ADP	PB-O2B	2.20	1.63	1.54
2	B	400	ADP	PA-O3A	2.15	1.61	1.59
4	A	403	PI	P-O2	-2.13	1.48	1.54
2	A	400	ADP	PB-O2B	2.10	1.62	1.54
2	B	400	ADP	C8-N7	2.01	1.35	1.31

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	ADP	C5-C4-N9	4.41	110.62	105.81
2	A	400	ADP	N3-C2-N1	-4.30	122.08	128.58
2	B	400	ADP	O4'-C4'-C3'	-3.88	97.44	105.15
2	B	400	ADP	C4'-O4'-C1'	3.60	117.42	109.47
2	B	400	ADP	C4-N9-C8	-2.99	102.60	105.74
4	B	403	PI	O4-P-O1	-2.89	100.74	110.95
4	B	403	PI	O4-P-O3	2.80	116.64	107.91
2	A	400	ADP	C5-C6-N6	2.72	130.01	123.29
2	B	400	ADP	C4-C5-N7	-2.71	107.48	110.58
2	B	400	ADP	C5-C6-N6	2.66	129.88	123.29
2	B	400	ADP	O4'-C1'-C2'	-2.66	100.93	106.62
2	A	400	ADP	N6-C6-N1	-2.60	112.58	118.38
2	B	400	ADP	O3A-PA-O1A	-2.57	102.98	110.70
2	A	400	ADP	C2'-C1'-N9	-2.48	107.15	113.30
2	B	400	ADP	C5-C4-N3	-2.46	123.33	126.72
2	B	400	ADP	N3-C2-N1	-2.42	124.92	128.58
2	B	400	ADP	O2A-PA-O5'	2.38	118.34	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	ADP	O4'-C1'-N9	-2.35	103.57	108.09
2	A	400	ADP	C2-N1-C6	2.33	122.56	118.73
2	B	400	ADP	O2A-PA-O3A	2.30	113.48	107.27
2	A	400	ADP	C4'-O4'-C1'	2.24	114.40	109.47
2	B	400	ADP	O3'-C3'-C2'	2.17	118.77	111.82
2	A	400	ADP	O3'-C3'-C2'	2.08	118.49	111.82
2	B	400	ADP	O2B-PB-O3A	2.03	111.45	104.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

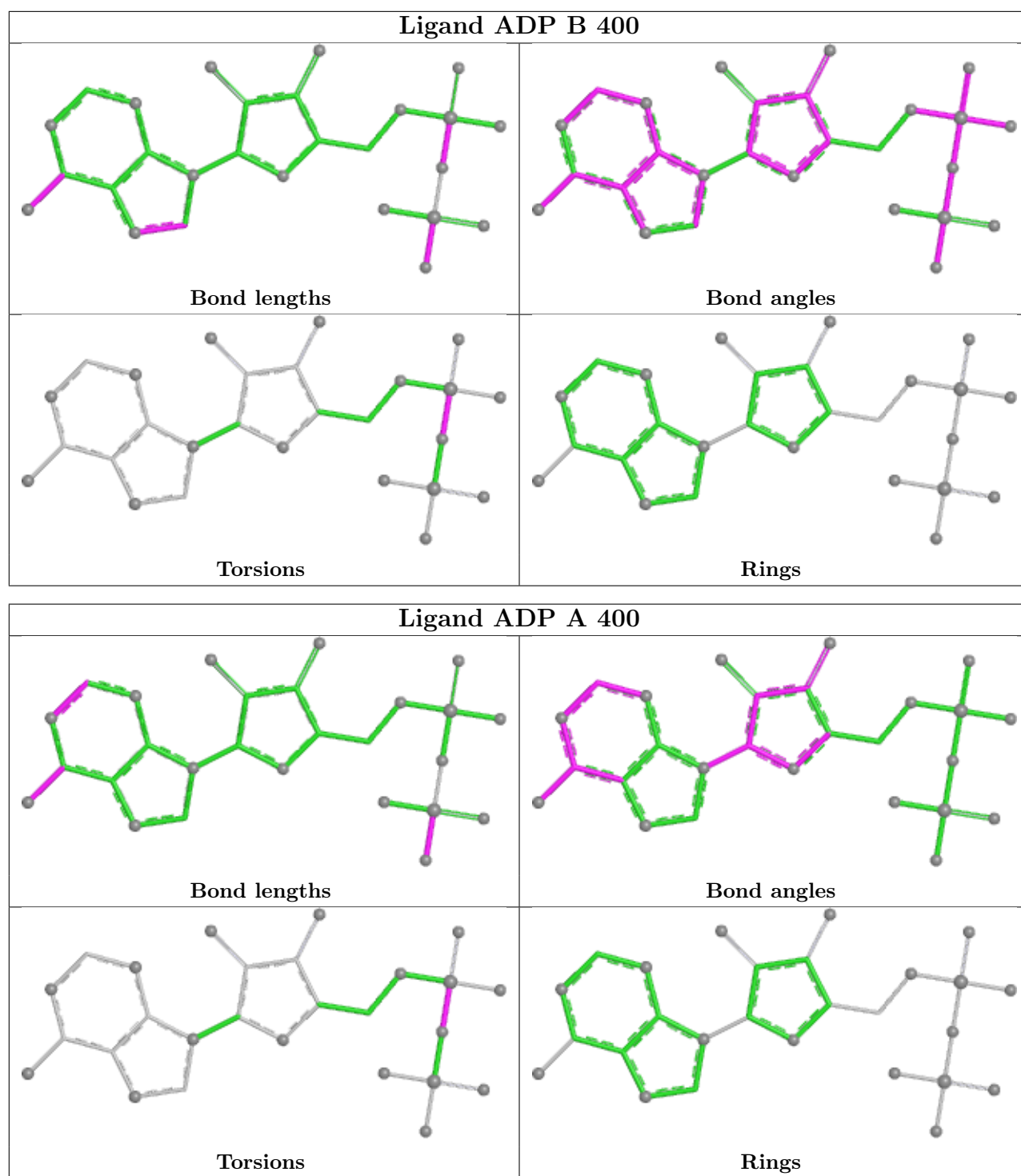
Mol	Chain	Res	Type	Atoms
2	A	400	ADP	PB-O3A-PA-O2A
2	B	400	ADP	PB-O3A-PA-O2A
2	A	400	ADP	PB-O3A-PA-O1A
2	B	400	ADP	PB-O3A-PA-O1A

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	ADP	1	0
4	B	403	PI	1	0
4	A	403	PI	1	0
2	A	400	ADP	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	355/355 (100%)	-0.52	2 (0%) 85 88	13, 20, 58, 90	2 (0%)
1	B	351/355 (98%)	-0.43	9 (2%) 57 60	13, 21, 63, 100	3 (0%)
All	All	706/710 (99%)	-0.48	11 (1%) 70 74	13, 21, 61, 100	5 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	VAL	5.9
1	B	125	GLY	4.6
1	B	37	ALA	4.4
1	B	41	PHE	2.9
1	A	28	TRP	2.8
1	B	124	GLY	2.8
1	A	126	TYR	2.6
1	B	1	MET	2.3
1	B	2	LYS	2.1
1	B	40	PRO	2.1
1	B	38	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

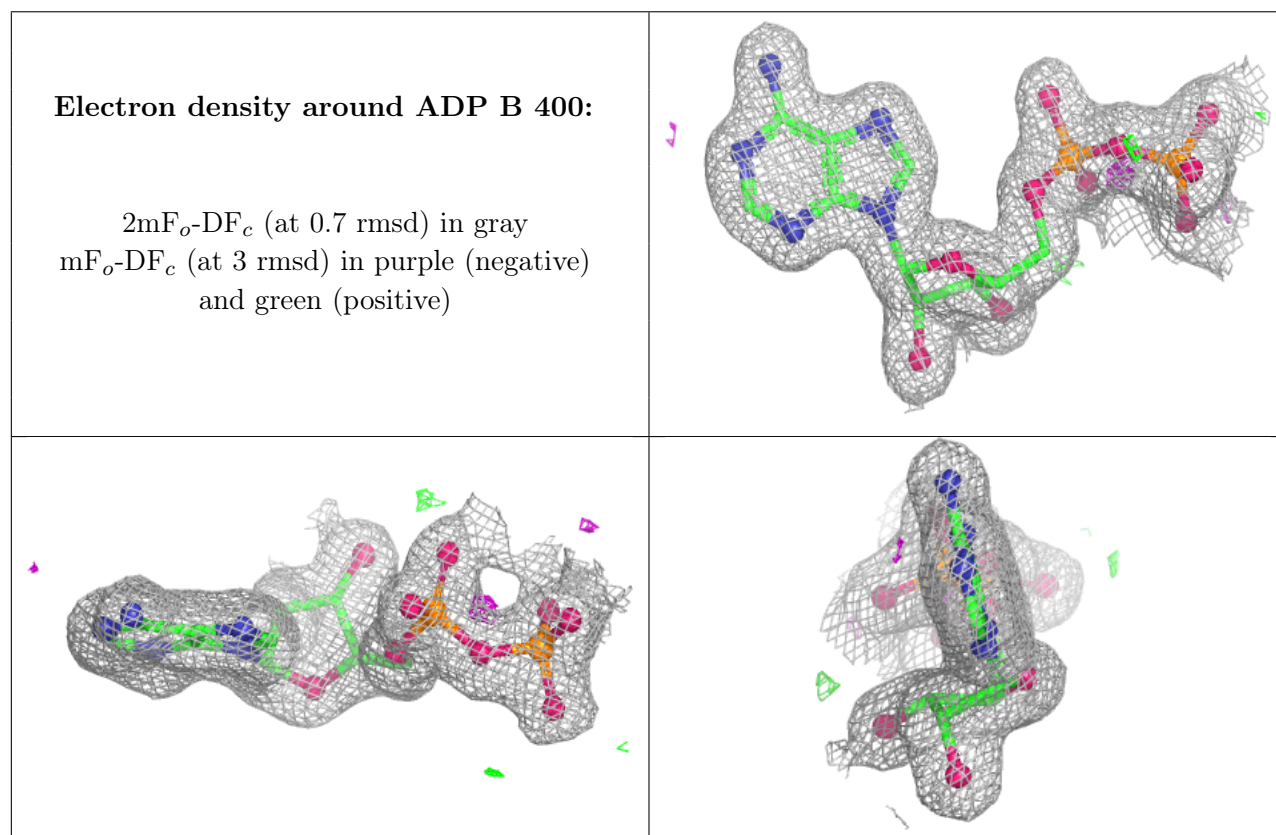
There are no oligosaccharides in this entry.

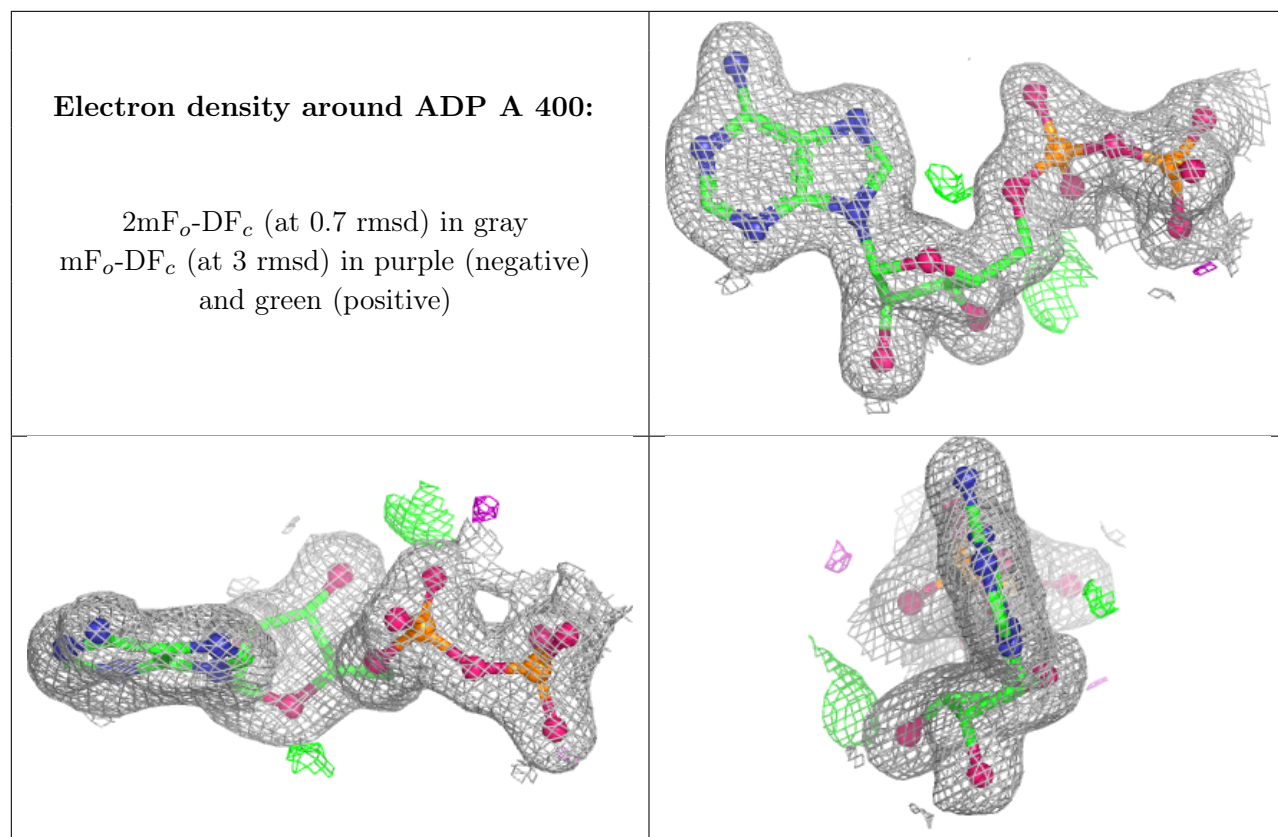
6.4 Ligands ⓘ

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
4	PI	B	403	5/5	0.92	0.10	28,32,37,99	0
2	ADP	B	400	27/27	0.98	0.04	15,21,32,47	0
5	CL	A	404	1/1	0.98	0.14	43,43,43,43	0
3	MG	A	402	1/1	0.99	0.02	18,18,18,18	0
3	MG	B	401	1/1	0.99	0.02	17,17,17,17	0
3	MG	B	402	1/1	0.99	0.05	25,25,25,25	0
4	PI	A	403	5/5	0.99	0.04	19,21,27,27	0
2	ADP	A	400	27/27	0.99	0.03	15,19,25,31	0
3	MG	A	401	1/1	0.99	0.02	15,15,15,15	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.