



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2021 – 06:05 PM EDT

PDB ID : 7RCL
Title : Crystal Structure of ADP-bound Galactokinase
Authors : Whitby, F.G.; Hall, M.D.
Deposited on : 2021-07-07
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

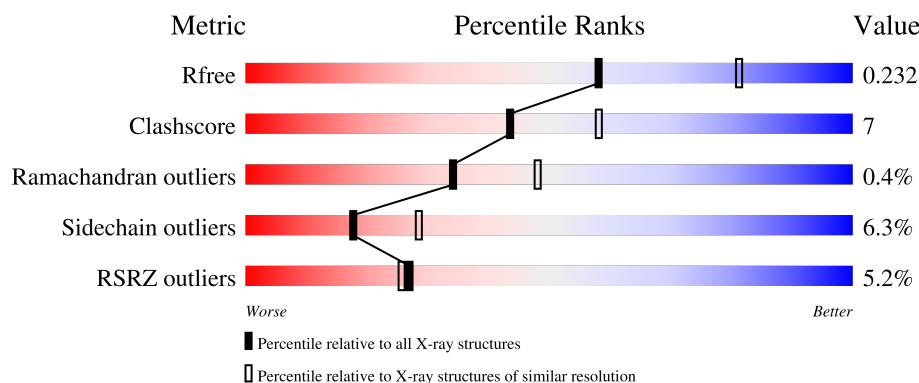
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	392	<div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	B	392	<div> <div>2%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
1	C	392	<div> <div>4%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	D	392	<div> <div>15%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>

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
5	MG	D	406	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12536 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.

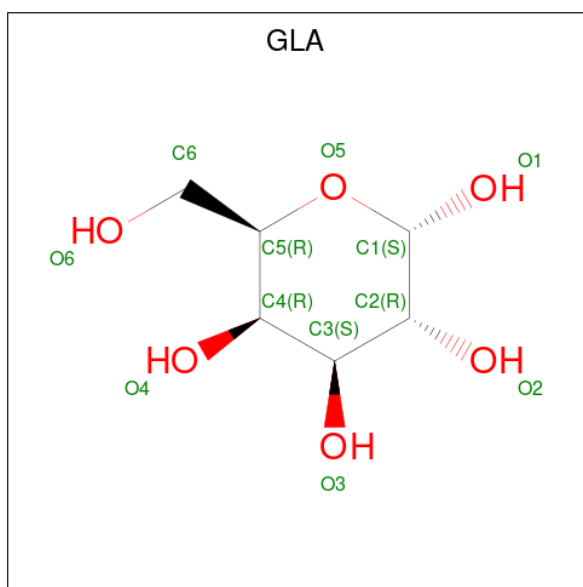
- Molecule 1 is a protein called Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	2	0
			2968	1851	538	563	16			
1	B	391	Total	C	N	O	S	0	11	0
			3034	1891	551	576	16			
1	C	391	Total	C	N	O	S	0	2	0
			2968	1851	538	563	16			
1	D	391	Total	C	N	O	S	0	0	0
			2950	1841	534	559	16			

There are 8 discrepancies between the modelled and reference sequences:

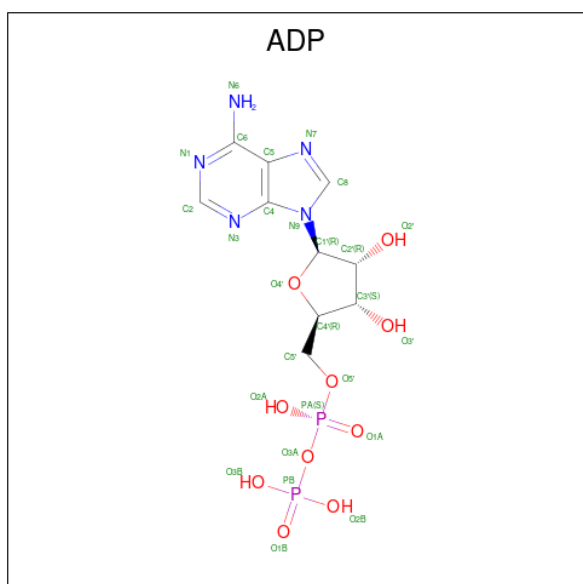
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ALA	LYS	engineered mutation	UNP P51570
A	253	ALA	GLU	engineered mutation	UNP P51570
B	252	ALA	LYS	engineered mutation	UNP P51570
B	253	ALA	GLU	engineered mutation	UNP P51570
C	252	ALA	LYS	engineered mutation	UNP P51570
C	253	ALA	GLU	engineered mutation	UNP P51570
D	252	ALA	LYS	engineered mutation	UNP P51570
D	253	ALA	GLU	engineered mutation	UNP P51570

- Molecule 2 is alpha-D-galactopyranose (three-letter code: GLA) (formula: C₆H₁₂O₆).



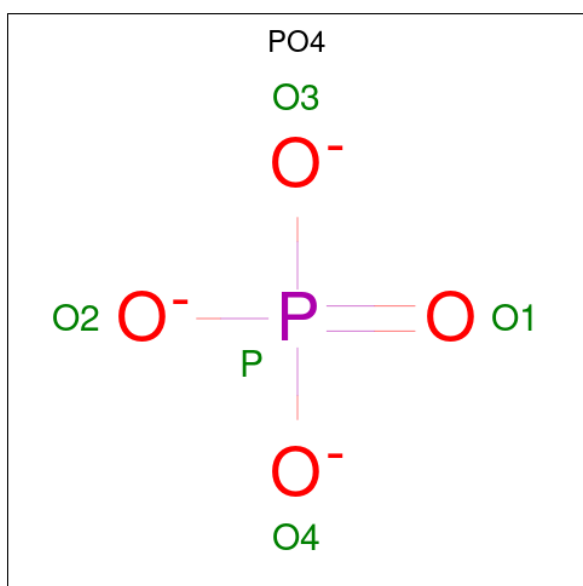
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

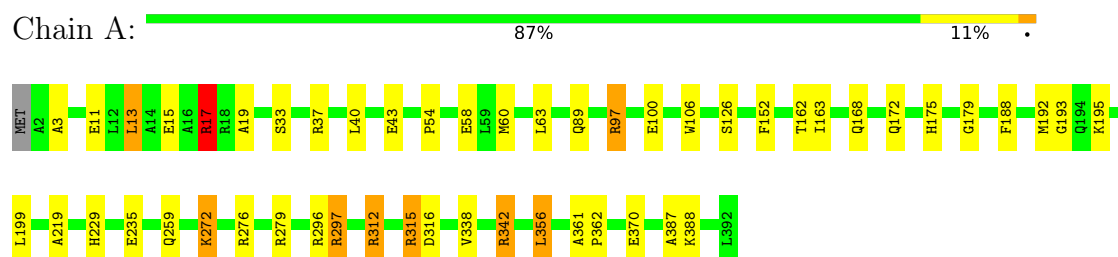
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	123	Total	O	0	0
			123	123		
7	B	110	Total	O	0	0
			110	110		
7	C	88	Total	O	0	0
			88	88		
7	D	76	Total	O	0	0
			76	76		

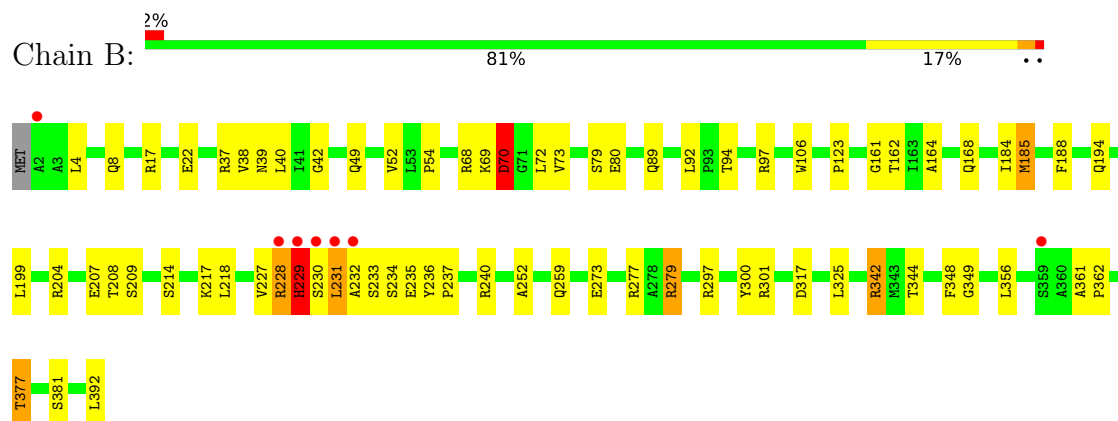
3 Residue-property plots

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.

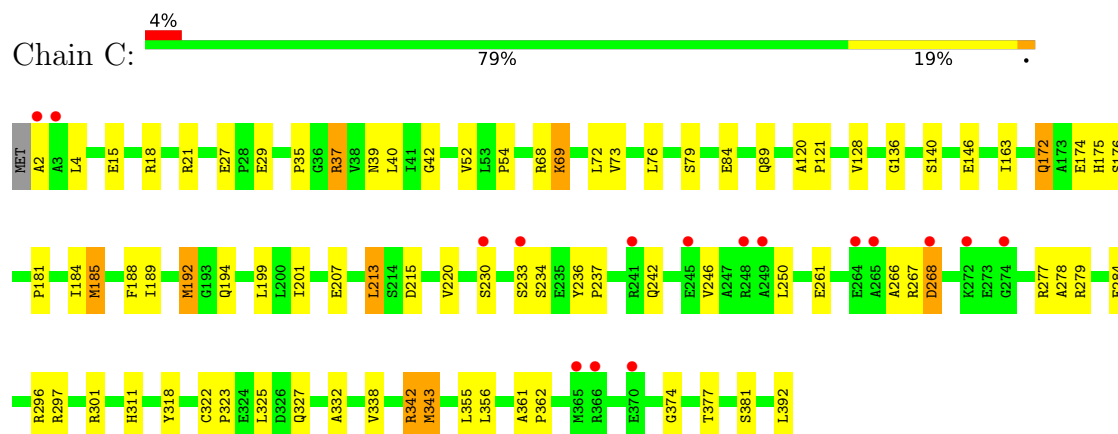
• Molecule 1: Galactokinase



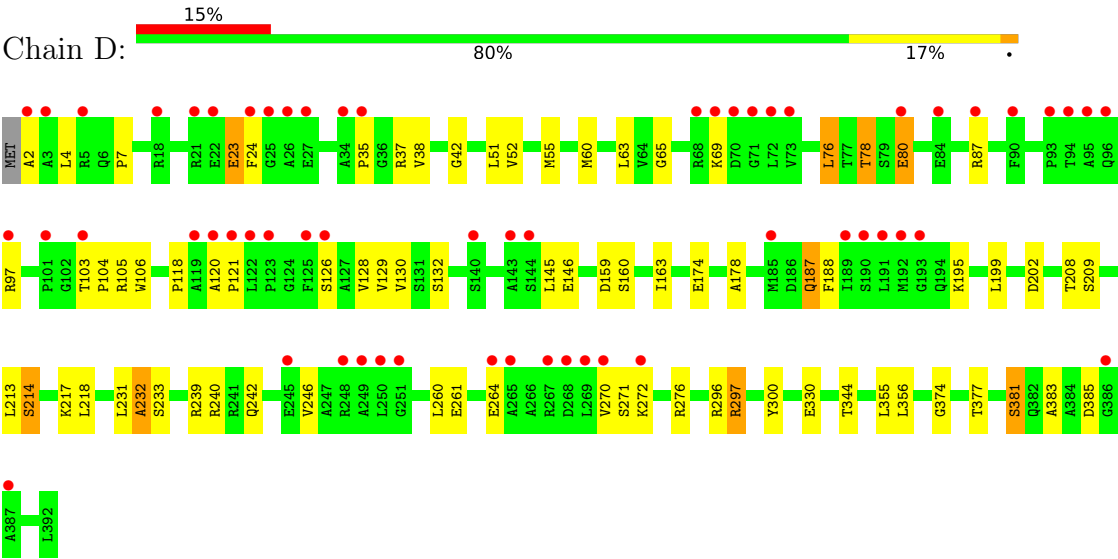
• Molecule 1: Galactokinase



• Molecule 1: Galactokinase



● Molecule 1: Galactokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.90Å 114.13Å 206.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.63 – 2.40 39.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.6 (39.63-2.40) 95.6 (39.63-2.40)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.173 , 0.228 0.178 , 0.232	Depositor DCC
R_{free} test set	1726 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12536	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: PO4, GLA, ADP, MG, NA

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	0.98	6/3022 (0.2%)	1.11	9/4098 (0.2%)
1	B	0.90	1/3089 (0.0%)	1.14	9/4189 (0.2%)
1	C	0.87	5/3022 (0.2%)	1.09	9/4098 (0.2%)
1	D	0.86	3/3004 (0.1%)	1.05	4/4074 (0.1%)
All	All	0.90	15/12137 (0.1%)	1.10	31/16459 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	5
1	D	0	3
All	All	0	10

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	GLU	CD-OE1	9.42	1.36	1.25
1	A	235	GLU	CD-OE1	9.20	1.35	1.25
1	A	58	GLU	CD-OE2	8.41	1.34	1.25
1	A	11	GLU	CD-OE1	7.29	1.33	1.25
1	D	330	GLU	CD-OE1	6.30	1.32	1.25
1	C	15	GLU	CD-OE1	5.64	1.31	1.25
1	C	261	GLU	CD-OE1	5.63	1.31	1.25
1	D	261	GLU	CD-OE1	5.52	1.31	1.25
1	A	370	GLU	CD-OE2	5.51	1.31	1.25
1	C	29	GLU	CD-OE2	5.46	1.31	1.25
1	C	207	GLU	CD-OE1	5.33	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	GLU	CD-OE2	5.32	1.31	1.25
1	D	374	GLY	C-O	5.25	1.32	1.23
1	A	15	GLU	CD-OE2	5.09	1.31	1.25
1	B	207	GLU	CD-OE1	5.07	1.31	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ARG	NE-CZ-NH1	11.89	126.25	120.30
1	B	70	ASP	CB-CG-OD1	-9.64	109.63	118.30
1	B	279	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	B	240	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	279	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	C	342	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	C	296	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	342	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	279	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	97	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	C	297	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	C	342	ARG	CG-CD-NE	-6.51	98.13	111.80
1	B	185	MET	CG-SD-CE	-6.46	89.86	100.20
1	B	240	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	315	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	D	297	ARG	CB-CA-C	5.67	121.73	110.40
1	A	297	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	342	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	D	239	ARG	CG-CD-NE	-5.62	100.00	111.80
1	C	68	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	297	ARG	CG-CD-NE	-5.53	100.19	111.80
1	B	70	ASP	CA-CB-CG	-5.51	101.28	113.40
1	C	215	ASP	CB-CA-C	5.44	121.27	110.40
1	C	185	MET	CG-SD-CE	-5.41	91.55	100.20
1	D	240	ARG	CG-CD-NE	-5.38	100.51	111.80
1	C	68	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	70	ASP	N-CA-CB	-5.30	101.06	110.60
1	A	296	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	17	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	296	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	296	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	229[A]	HIS	Peptide
1	B	94	THR	Peptide
1	C	2	ALA	Peptide
1	C	233	SER	Peptide
1	C	35	PRO	Peptide
1	C	72	LEU	Mainchain
1	C	79	SER	Peptide
1	D	2	ALA	Peptide
1	D	233	SER	Peptide
1	D	80	GLU	Peptide

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	2968	0	2959	25	0
1	B	3034	0	3025	51	0
1	C	2968	0	2959	44	0
1	D	2950	0	2945	45	0
2	A	12	0	11	0	0
2	B	12	0	11	0	0
2	C	12	0	11	0	0
2	D	12	0	11	0	0
3	A	27	0	12	1	0
3	B	27	0	12	2	0
3	C	27	0	12	2	0
3	D	27	0	12	1	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	123	0	0	4	0
7	B	110	0	0	6	0
7	C	88	0	0	4	0
7	D	76	0	0	4	0
All	All	12536	0	11980	162	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 7.

All (162) 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:78:THR:HG21	1:D:130:VAL:HG22	1.32	1.06
1:D:55:MET:HE2	1:D:383:ALA:HB2	1.47	0.94
1:C:52:VAL:HB	1:C:185:MET:CE	1.99	0.92
1:D:55:MET:CE	1:D:213:LEU:HD23	2.04	0.87
1:D:218:LEU:HD11	1:D:355:LEU:HD22	1.57	0.86
1:C:325:LEU:HD13	1:C:343:MET:HG3	1.58	0.84
1:D:63:LEU:HD11	1:D:129:VAL:HG22	1.60	0.84
1:D:78:THR:CG2	1:D:130:VAL:HG22	2.09	0.83
1:B:229[A]:HIS:O	1:B:232[A]:ALA:HB2	1.82	0.80
1:D:120:ALA:HB1	1:D:121:PRO:HA	1.65	0.79
1:C:52:VAL:HB	1:C:185:MET:HE3	1.67	0.76
1:A:17:ARG:HH11	1:A:17:ARG:HG3	1.52	0.75
1:C:4:LEU:HD13	1:C:377:THR:HG23	1.70	0.74
1:C:52:VAL:HB	1:C:185:MET:HE1	1.70	0.73
1:B:79:SER:OG	7:B:501:HOH:O	2.06	0.72
1:D:218:LEU:HD11	1:D:355:LEU:CD2	2.19	0.71
1:B:4:LEU:HD13	1:B:377:THR:CG2	2.25	0.67
1:B:252:ALA:O	7:B:502:HOH:O	2.13	0.66
1:A:315:ARG:HD2	1:A:316:ASP:OD1	1.96	0.66
1:D:105:ARG:HB2	1:D:105:ARG:CZ	2.26	0.66
1:B:279:ARG:HD2	1:B:317:ASP:OD2	1.96	0.66
1:B:231[B]:LEU:O	1:B:234[B]:SER:OG	2.11	0.66
3:C:402:ADP:O3B	7:C:501:HOH:O	2.12	0.66
1:C:54:PRO:HD2	1:C:199:LEU:O	1.96	0.66
1:D:78:THR:HG22	1:D:129:VAL:O	1.97	0.65
1:D:55:MET:HE3	1:D:213:LEU:HD23	1.78	0.65
1:C:381:SER:HB2	7:C:560:HOH:O	1.97	0.63
1:A:17:ARG:HH11	1:A:17:ARG:CG	2.12	0.63
1:C:246:VAL:O	1:C:250:LEU:HD13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:PHE:HE1	1:D:208:THR:HG21	1.63	0.63
1:B:188:PHE:CE1	1:B:208:THR:HG21	2.36	0.60
1:D:63:LEU:CD1	1:D:129:VAL:HG22	2.30	0.60
1:B:188:PHE:HE1	1:B:208:THR:HG21	1.66	0.59
1:D:163:ILE:HD12	1:D:163:ILE:H	1.67	0.59
1:A:54:PRO:HD2	1:A:199:LEU:O	2.03	0.59
1:A:361:ALA:HB3	1:A:362:PRO:HD3	1.85	0.58
1:D:55:MET:HE3	1:D:213:LEU:CD2	2.34	0.58
1:D:60:MET:HE1	7:D:506:HOH:O	2.03	0.58
1:C:381:SER:CB	7:C:560:HOH:O	2.51	0.58
1:A:312:ARG:NE	7:A:504:HOH:O	2.37	0.56
1:D:55:MET:CE	1:D:213:LEU:CD2	2.79	0.56
1:D:4:LEU:CD1	1:D:377:THR:HG23	2.36	0.56
1:D:4:LEU:HD11	1:D:377:THR:HG23	1.87	0.56
1:D:76:LEU:HD23	1:D:128:VAL:HG13	1.87	0.56
1:C:172[B]:GLN:NE2	1:C:176:SER:OG	2.37	0.56
1:B:230[A]:SER:C	1:B:232[A]:ALA:N	2.58	0.55
1:C:69:LYS:N	1:C:69:LYS:HD3	2.21	0.55
1:B:233[A]:SER:O	1:B:234[A]:SER:HB3	2.06	0.55
1:C:246:VAL:HG11	1:C:278:ALA:HB2	1.89	0.55
1:D:276:ARG:HD3	7:D:505:HOH:O	2.06	0.54
1:B:218:LEU:HD22	1:B:300:TYR:CE1	2.42	0.54
1:C:175:HIS:CD2	1:C:181:PRO:HA	2.43	0.54
1:C:242:GLN:O	1:C:246:VAL:HG23	2.08	0.54
1:A:168[B]:GLN:NE2	1:A:172[B]:GLN:OE1	2.41	0.53
1:C:73:VAL:O	1:C:89:GLN:HA	2.07	0.53
1:B:54:PRO:HB3	1:B:185:MET:CE	2.39	0.53
1:B:49[B]:GLN:HG2	1:B:204:ARG:HA	1.90	0.53
1:C:120:ALA:HB1	1:C:121:PRO:HA	1.91	0.53
1:D:55:MET:HE1	1:D:213:LEU:HD23	1.86	0.53
1:D:42:GLY:O	1:D:52:VAL:HG12	2.09	0.52
1:A:33:SER:O	1:A:387:ALA:HA	2.09	0.52
1:B:229[A]:HIS:O	1:B:232[A]:ALA:CB	2.55	0.52
1:C:361:ALA:HB3	1:C:362:PRO:HD3	1.91	0.52
1:C:52:VAL:CB	1:C:185:MET:HE3	2.38	0.52
1:B:54:PRO:HD2	1:B:199:LEU:O	2.10	0.52
1:C:146:GLU:OE2	1:C:174:GLU:OE1	2.27	0.52
1:C:42:GLY:O	1:C:52:VAL:HG12	2.10	0.51
1:B:106:TRP:HB2	3:B:402:ADP:N3	2.25	0.51
1:D:78:THR:CG2	1:D:130:VAL:HA	2.41	0.51
1:C:52:VAL:CB	1:C:185:MET:CE	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227[A]:VAL:HG12	1:B:228[A]:ARG:N	2.26	0.50
1:B:228[B]:ARG:NH2	3:B:402:ADP:O1B	2.44	0.50
1:D:231:LEU:O	1:D:232:ALA:C	2.49	0.50
1:D:381:SER:HB3	7:D:534:HOH:O	2.11	0.50
1:A:219:ALA:HB3	1:A:356:LEU:CD1	2.42	0.50
1:B:361:ALA:HB3	1:B:362:PRO:HD3	1.94	0.50
1:B:381:SER:HB3	7:B:583:HOH:O	2.11	0.49
1:C:311:HIS:HB2	1:C:342:ARG:HB3	1.93	0.49
1:B:39:ASN:OD1	1:B:185:MET:HE3	2.12	0.49
1:B:232[A]:ALA:HA	1:B:348:PHE:CB	2.42	0.49
1:C:268:ASP:N	1:C:268:ASP:OD1	2.46	0.49
1:D:7:PRO:HG2	1:D:132:SER:HB3	1.95	0.49
1:D:106:TRP:HB2	3:D:402:ADP:N3	2.28	0.49
1:A:17:ARG:HG3	1:A:17:ARG:NH1	2.18	0.49
1:B:4:LEU:HD13	1:B:377:THR:HG22	1.95	0.48
1:A:43:GLU:HB2	1:A:342:ARG:NH2	2.29	0.48
1:D:103:THR:HA	1:D:104:PRO:C	2.35	0.47
1:A:3:ALA:HB1	7:A:534:HOH:O	2.14	0.47
1:B:227[A]:VAL:HG12	1:B:228[A]:ARG:H	1.80	0.47
1:A:312:ARG:CD	7:A:504:HOH:O	2.63	0.47
1:B:68:ARG:HB3	1:B:70:ASP:HB2	1.97	0.46
1:D:218:LEU:HD22	1:D:300:TYR:CE1	2.50	0.46
1:D:260:LEU:O	1:D:264:GLU:HG2	2.15	0.46
1:B:49[A]:GLN:NE2	7:B:507:HOH:O	2.47	0.46
1:C:213:LEU:HD12	1:C:213:LEU:C	2.36	0.46
1:D:188:PHE:CE1	1:D:208:THR:HG21	2.48	0.46
1:B:325:LEU:HD11	1:B:349:GLY:O	2.15	0.46
1:B:208:THR:HG23	7:B:577:HOH:O	2.16	0.46
1:D:214:SER:HB2	7:D:541:HOH:O	2.16	0.46
1:A:259:GLN:NE2	1:B:259:GLN:CD	2.69	0.46
1:A:106:TRP:HB2	3:A:402:ADP:N3	2.30	0.46
1:A:338:VAL:HA	1:A:356:LEU:HB3	1.98	0.46
1:B:162:THR:HB	7:B:561:HOH:O	2.17	0.45
1:B:230[A]:SER:C	1:B:232[A]:ALA:H	2.17	0.45
1:C:311:HIS:HB2	1:C:342:ARG:CB	2.46	0.45
1:C:220:VAL:HG22	1:C:355:LEU:HD12	1.97	0.45
1:A:19:ALA:O	7:A:501:HOH:O	2.21	0.45
1:A:272:LYS:HG2	1:A:276:ARG:HH11	1.82	0.45
1:D:38:VAL:HG23	1:D:344:THR:HG21	1.99	0.45
1:B:40:LEU:O	1:B:342:ARG:HD3	2.17	0.45
1:B:297:ARG:O	1:B:297:ARG:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLY:O	1:B:52:VAL:HG12	2.17	0.45
1:C:39:ASN:OD1	1:C:185:MET:HE2	2.17	0.45
1:B:39:ASN:CG	1:B:185:MET:CE	2.85	0.44
1:C:236:TYR:HB3	1:C:237:PRO:HD3	1.99	0.44
1:C:42:GLY:HA2	1:C:284:GLU:HG3	1.99	0.44
1:A:259:GLN:HG2	1:B:259:GLN:OE1	2.16	0.44
1:C:40:LEU:HD11	1:C:213:LEU:HD23	2.00	0.44
1:C:184:ILE:O	1:C:188:PHE:HB2	2.17	0.44
1:A:40:LEU:O	1:A:342:ARG:HD3	2.18	0.44
1:D:187:GLN:NE2	1:D:187:GLN:H	2.15	0.44
1:B:54:PRO:HB3	1:B:185:MET:HE1	1.99	0.44
1:B:273:GLU:O	1:B:277:ARG:HG2	2.18	0.43
1:C:69:LYS:HE3	7:C:578:HOH:O	2.17	0.43
1:B:236:TYR:N	1:B:237:PRO:HD2	2.34	0.43
1:D:146:GLU:OE2	1:D:174:GLU:OE1	2.35	0.43
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.85	0.43
1:B:70:ASP:HB3	1:B:72:LEU:H	1.84	0.43
1:D:35:PRO:HG3	1:D:385:ASP:O	2.18	0.43
1:C:39:ASN:ND2	1:C:185:MET:HE1	2.34	0.43
1:C:54:PRO:HB3	1:C:185:MET:HE2	2.01	0.42
1:B:184:ILE:HD12	1:B:184:ILE:HA	1.88	0.42
1:D:356:LEU:HD23	1:D:356:LEU:N	2.34	0.42
1:B:39:ASN:CG	1:B:185:MET:HE3	2.40	0.42
1:B:161:GLY:O	1:D:195:LYS:HE3	2.19	0.42
1:D:51:LEU:HD23	1:D:202:ASP:HA	2.00	0.42
1:D:65:GLY:CA	1:D:126:SER:O	2.68	0.42
1:C:37:ARG:C	1:C:37:ARG:HD2	2.40	0.42
1:B:392:LEU:HD23	1:B:392:LEU:HA	1.89	0.42
1:C:52:VAL:CG2	1:C:201:ILE:HB	2.50	0.42
1:B:52:VAL:HB	1:B:185:MET:HE3	2.00	0.41
1:D:24:PHE:CE1	1:D:126:SER:HB3	2.55	0.41
1:C:136:GLY:HA2	3:C:402:ADP:O3A	2.19	0.41
1:B:4:LEU:HD13	1:B:377:THR:HG23	2.02	0.41
1:B:92:LEU:HD11	1:B:123:PRO:C	2.41	0.41
1:B:164:ALA:O	1:B:168:GLN:HG3	2.21	0.41
1:C:37:ARG:HG2	1:C:189:ILE:HG21	2.02	0.41
1:C:39:ASN:CG	1:C:185:MET:CE	2.88	0.41
1:A:63:LEU:HD22	1:A:152:PHE:CD1	2.56	0.41
1:C:76:LEU:O	1:C:128:VAL:HA	2.21	0.41
1:C:163:ILE:HG21	1:C:192:MET:SD	2.60	0.41
1:C:322:CYS:HB2	1:C:323:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:GLU:O	1:D:178:ALA:HB3	2.21	0.41
1:B:38:VAL:HG23	1:B:344:THR:HG21	2.01	0.41
1:B:233[A]:SER:O	1:B:234[A]:SER:CB	2.69	0.41
1:C:332:ALA:O	1:C:338:VAL:HG21	2.20	0.41
1:A:356:LEU:HD12	1:A:356:LEU:N	2.36	0.40
1:B:73:VAL:O	1:B:89:GLN:HA	2.22	0.40
1:A:163:ILE:HD12	1:C:194[B]:GLN:HG2	2.02	0.40
1:D:78:THR:HG23	1:D:130:VAL:HA	2.04	0.40
1:D:242:GLN:O	1:D:246:VAL:HG23	2.21	0.40
1:A:175:HIS:O	1:A:179:GLY:HA2	2.20	0.40

There are no symmetry-related clashes.

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	391/392 (100%)	381 (97%)	9 (2%)	1 (0%)	41	55
1	B	400/392 (102%)	383 (96%)	15 (4%)	2 (0%)	29	41
1	C	391/392 (100%)	374 (96%)	15 (4%)	2 (0%)	29	41
1	D	389/392 (99%)	371 (95%)	15 (4%)	3 (1%)	19	29
All	All	1571/1568 (100%)	1509 (96%)	54 (3%)	8 (0%)	34	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	232	ALA
1	C	374	GLY
1	A	193	GLY
1	D	271	SER
1	C	266	ALA

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Mol	Chain	Res	Type
1	D	23	GLU
1	B	228[A]	ARG
1	B	228[B]	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/309 (100%)	293 (94%)	17 (6%)	21	35
1	B	318/309 (103%)	297 (93%)	21 (7%)	16	26
1	C	310/309 (100%)	287 (93%)	23 (7%)	13	22
1	D	308/309 (100%)	287 (93%)	21 (7%)	16	25
All	All	1246/1236 (101%)	1164 (93%)	82 (7%)	18	26

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	17	ARG
1	A	37	ARG
1	A	60	MET
1	A	89	GLN
1	A	97	ARG
1	A	126	SER
1	A	162	THR
1	A	188	PHE
1	A	192	MET
1	A	195	LYS
1	A	229	HIS
1	A	272	LYS
1	A	297	ARG
1	A	312	ARG
1	A	356	LEU
1	A	388	LYS
1	B	8	GLN

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Mol	Chain	Res	Type
1	B	17	ARG
1	B	22	GLU
1	B	37	ARG
1	B	69	LYS
1	B	70	ASP
1	B	80	GLU
1	B	97	ARG
1	B	194	GLN
1	B	209	SER
1	B	214	SER
1	B	217	LYS
1	B	229[A]	HIS
1	B	229[B]	HIS
1	B	231[A]	LEU
1	B	231[B]	LEU
1	B	235[A]	GLU
1	B	235[B]	GLU
1	B	301	ARG
1	B	356	LEU
1	B	377	THR
1	C	18	ARG
1	C	21	ARG
1	C	27	GLU
1	C	37	ARG
1	C	69	LYS
1	C	84	GLU
1	C	140	SER
1	C	172[A]	GLN
1	C	172[B]	GLN
1	C	192	MET
1	C	213	LEU
1	C	230	SER
1	C	234	SER
1	C	267	ARG
1	C	268	ASP
1	C	277	ARG
1	C	279	ARG
1	C	301	ARG
1	C	318	TYR
1	C	327	GLN
1	C	343	MET
1	C	356	LEU

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Mol	Chain	Res	Type
1	C	392	LEU
1	D	23	GLU
1	D	37	ARG
1	D	69	LYS
1	D	76	LEU
1	D	78	THR
1	D	80	GLU
1	D	87	ARG
1	D	97	ARG
1	D	118	PRO
1	D	145	LEU
1	D	159	ASP
1	D	160	SER
1	D	187	GLN
1	D	199	LEU
1	D	209	SER
1	D	214	SER
1	D	217	LYS
1	D	270	VAL
1	D	272	LYS
1	D	297	ARG
1	D	381	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	242	GLN
1	A	259	GLN
1	B	8	GLN
1	B	172	GLN
1	B	242	GLN
1	C	290	GLN
1	C	327	GLN
1	C	367	HIS
1	D	89	GLN
1	D	168	GLN
1	D	187	GLN
1	D	371	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 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	GLA	C	401	-	12,12,12	3.23	6 (50%)	17,17,17	2.08	7 (41%)
2	GLA	B	401	-	12,12,12	2.67	5 (41%)	17,17,17	2.18	4 (23%)
4	PO4	D	404	-	4,4,4	1.06	0	6,6,6	0.34	0
4	PO4	D	403	-	4,4,4	0.72	0	6,6,6	0.45	0
4	PO4	C	404	-	4,4,4	0.69	0	6,6,6	0.47	0
4	PO4	C	403	-	4,4,4	0.79	0	6,6,6	0.44	0
4	PO4	B	404	-	4,4,4	0.67	0	6,6,6	0.48	0
4	PO4	D	405	-	4,4,4	0.78	0	6,6,6	0.42	0
4	PO4	B	403	-	4,4,4	1.03	0	6,6,6	0.38	0
2	GLA	D	401	-	12,12,12	3.00	4 (33%)	17,17,17	2.05	5 (29%)
3	ADP	B	402	5	24,29,29	0.70	0	29,45,45	0.96	1 (3%)
4	PO4	B	405	-	4,4,4	0.48	0	6,6,6	0.68	0
4	PO4	A	404	-	4,4,4	0.67	0	6,6,6	0.49	0
3	ADP	A	402	5	24,29,29	0.79	0	29,45,45	1.07	2 (6%)
4	PO4	A	405	-	4,4,4	0.74	0	6,6,6	0.52	0
4	PO4	A	403	-	4,4,4	0.97	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	C	402	5	24,29,29	0.69	0	29,45,45	0.94	2 (6%)
3	ADP	D	402	-	24,29,29	0.67	1 (4%)	29,45,45	0.85	1 (3%)
2	GLA	A	401	-	12,12,12	2.80	8 (66%)	17,17,17	1.88	5 (29%)

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	GLA	C	401	-	-	2/2/22/22	0/1/1/1
2	GLA	B	401	-	-	2/2/22/22	0/1/1/1
2	GLA	D	401	-	-	1/2/22/22	0/1/1/1
3	ADP	B	402	5	-	3/12/32/32	0/3/3/3
3	ADP	C	402	5	-	3/12/32/32	0/3/3/3
3	ADP	D	402	-	-	7/12/32/32	0/3/3/3
2	GLA	A	401	-	-	1/2/22/22	0/1/1/1
3	ADP	A	402	5	-	2/12/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	GLA	O5-C1	-6.06	1.27	1.42
2	D	401	GLA	O3-C3	-6.04	1.28	1.43
2	C	401	GLA	O3-C3	-5.63	1.29	1.43
2	D	401	GLA	O5-C1	-5.29	1.29	1.42
2	A	401	GLA	O3-C3	-5.29	1.30	1.43
2	D	401	GLA	O5-C5	-5.08	1.32	1.44
2	B	401	GLA	O5-C5	-4.94	1.32	1.44
2	B	401	GLA	O5-C1	-4.47	1.31	1.42
2	C	401	GLA	O5-C5	-4.34	1.33	1.44
2	B	401	GLA	O3-C3	-4.31	1.32	1.43
2	A	401	GLA	O5-C5	-4.07	1.34	1.44
2	A	401	GLA	O5-C1	-3.82	1.33	1.42
2	A	401	GLA	O1-C1	3.41	1.50	1.39
2	C	401	GLA	C4-C3	3.01	1.60	1.52
2	C	401	GLA	C1-C2	2.98	1.59	1.52
2	D	401	GLA	O1-C1	2.80	1.48	1.39
2	C	401	GLA	O1-C1	2.66	1.48	1.39
2	A	401	GLA	C4-C3	2.45	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GLA	C6-C5	2.45	1.60	1.51
2	A	401	GLA	C1-C2	2.29	1.57	1.52
2	B	401	GLA	C3-C2	2.21	1.58	1.52
2	B	401	GLA	O2-C2	-2.18	1.37	1.43
2	A	401	GLA	C3-C2	2.14	1.57	1.52
3	D	402	ADP	C8-N7	-2.09	1.31	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GLA	C1-O5-C5	5.59	124.21	113.66
2	D	401	GLA	C1-O5-C5	5.46	123.96	113.66
2	B	401	GLA	C4-C3-C2	-5.09	101.93	110.82
2	C	401	GLA	C1-O5-C5	4.70	122.52	113.66
2	A	401	GLA	C1-O5-C5	4.18	121.56	113.66
2	A	401	GLA	C4-C3-C2	-3.71	104.34	110.82
2	D	401	GLA	C1-C2-C3	3.42	117.41	110.31
2	A	401	GLA	O2-C2-C3	-3.34	102.64	110.35
2	C	401	GLA	C4-C3-C2	-3.05	105.49	110.82
2	D	401	GLA	C4-C3-C2	-2.90	105.76	110.82
2	C	401	GLA	O4-C4-C3	2.87	116.98	110.35
2	C	401	GLA	C1-C2-C3	2.70	115.91	110.31
2	C	401	GLA	O3-C3-C4	2.56	116.27	110.35
2	A	401	GLA	O5-C5-C6	2.55	112.77	106.44
2	C	401	GLA	O2-C2-C3	-2.52	104.52	110.35
3	A	402	ADP	O3'-C3'-C4'	-2.46	103.95	111.05
3	B	402	ADP	O3B-PB-O3A	2.45	112.85	104.64
2	B	401	GLA	C1-C2-C3	2.37	115.24	110.31
2	C	401	GLA	O5-C5-C6	2.32	112.21	106.44
2	D	401	GLA	O3-C3-C2	-2.32	104.98	110.35
3	D	402	ADP	C5-C6-N6	2.25	123.78	120.35
3	C	402	ADP	C5-C6-N6	2.24	123.76	120.35
2	D	401	GLA	O2-C2-C3	-2.23	105.19	110.35
2	B	401	GLA	O5-C5-C6	2.19	111.87	106.44
2	A	401	GLA	O2-C2-C1	2.15	114.16	109.16
3	C	402	ADP	PA-O3A-PB	-2.10	125.62	132.83
3	A	402	ADP	C5-C6-N6	2.08	123.51	120.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

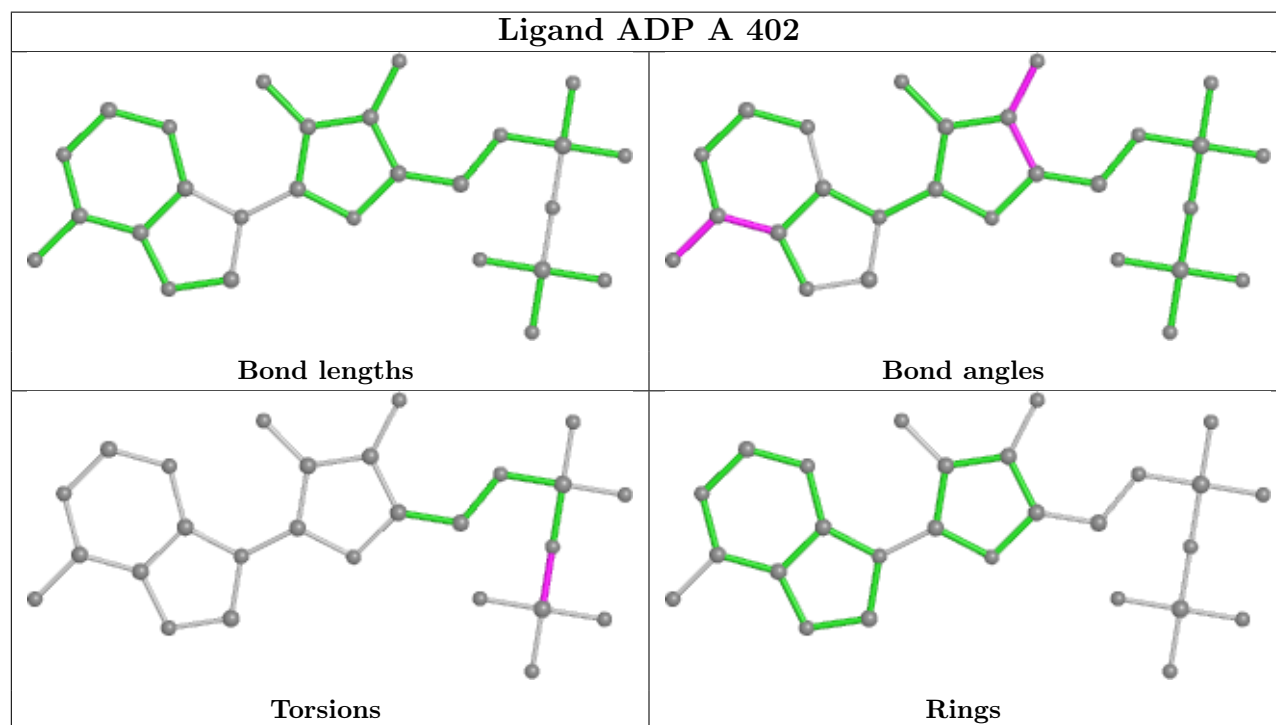
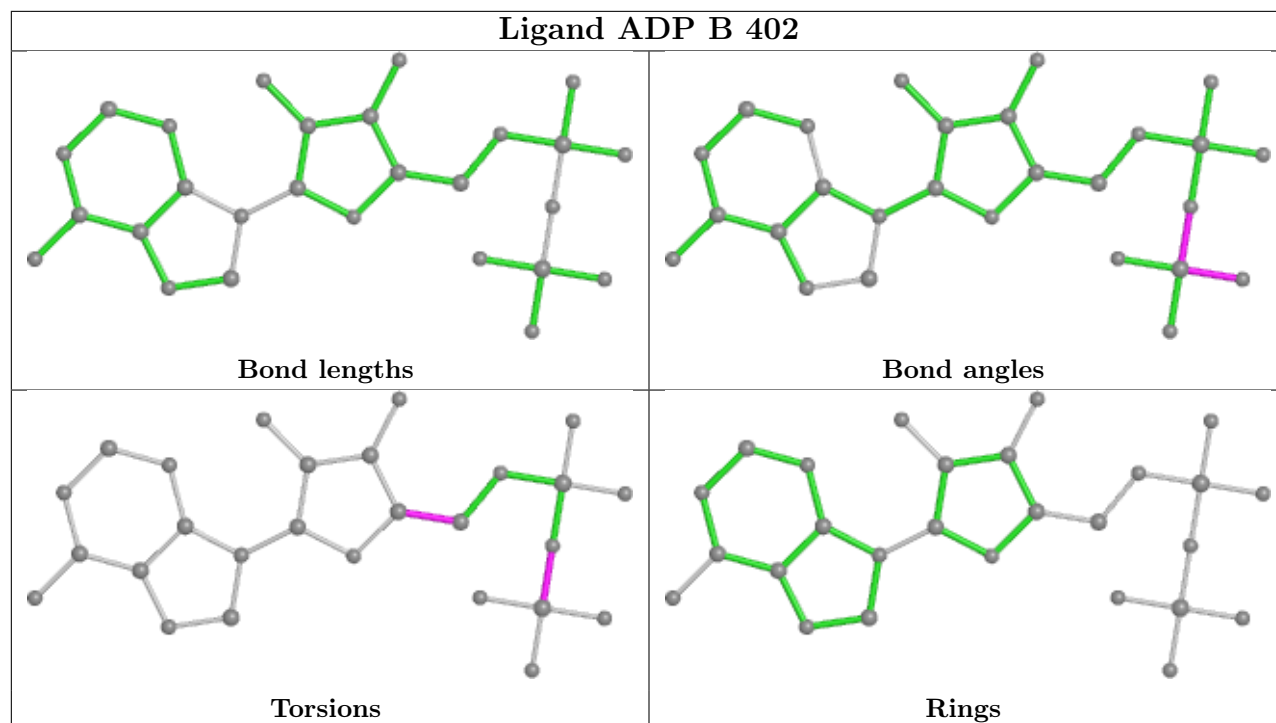
Mol	Chain	Res	Type	Atoms
3	B	402	ADP	PA-O3A-PB-O2B
3	C	402	ADP	PA-O3A-PB-O2B
3	C	402	ADP	PA-O3A-PB-O3B
3	D	402	ADP	PA-O3A-PB-O2B
2	C	401	GLA	O5-C5-C6-O6
3	D	402	ADP	O4'-C4'-C5'-O5'
3	D	402	ADP	C3'-C4'-C5'-O5'
2	B	401	GLA	O5-C5-C6-O6
2	A	401	GLA	O5-C5-C6-O6
2	C	401	GLA	C4-C5-C6-O6
2	D	401	GLA	O5-C5-C6-O6
2	B	401	GLA	C4-C5-C6-O6
3	A	402	ADP	PA-O3A-PB-O1B
3	A	402	ADP	PA-O3A-PB-O2B
3	D	402	ADP	PA-O3A-PB-O3B
3	D	402	ADP	PB-O3A-PA-O2A
3	B	402	ADP	C3'-C4'-C5'-O5'
3	C	402	ADP	PA-O3A-PB-O1B
3	D	402	ADP	PA-O3A-PB-O1B
3	B	402	ADP	PA-O3A-PB-O3B
3	D	402	ADP	PB-O3A-PA-O1A

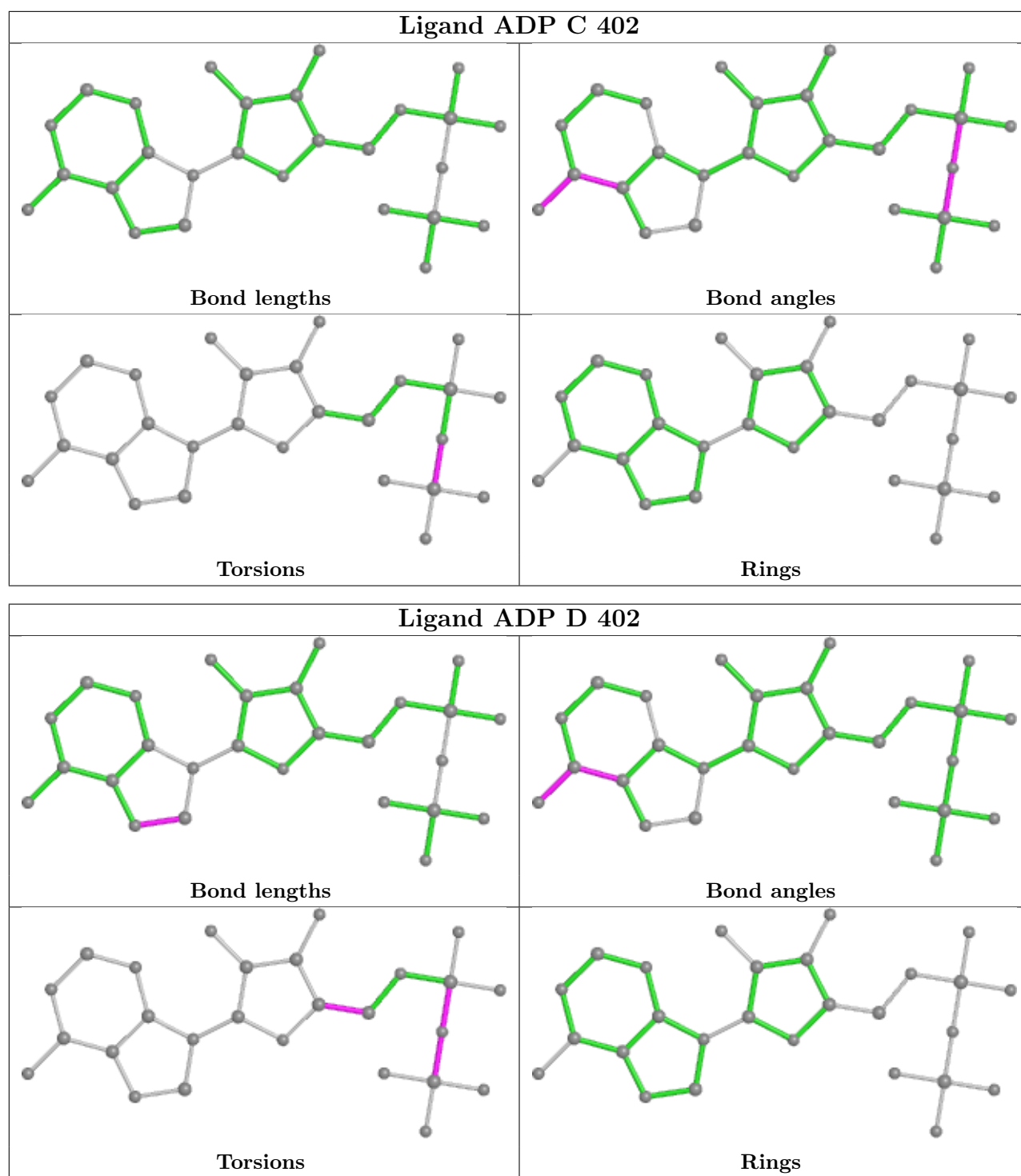
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	ADP	2	0
3	A	402	ADP	1	0
3	C	402	ADP	2	0
3	D	402	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

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	391/392 (99%)	-0.51	0 100 100	33, 50, 77, 104	0
1	B	391/392 (99%)	-0.21	7 (1%) 68 66	37, 51, 77, 95	0
1	C	391/392 (99%)	-0.05	16 (4%) 37 36	40, 60, 101, 145	0
1	D	391/392 (99%)	0.48	59 (15%) 2 1	41, 67, 109, 146	0
All	All	1564/1568 (99%)	-0.07	82 (5%) 27 26	33, 56, 98, 146	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	69	LYS	5.8
1	B	229[A]	HIS	5.5
1	C	2	ALA	4.7
1	D	269	LEU	4.7
1	D	265	ALA	4.6
1	B	231[A]	LEU	4.6
1	C	272	LYS	4.5
1	D	121	PRO	4.2
1	D	95	ALA	3.8
1	D	120	ALA	3.8
1	C	248	ARG	3.7
1	D	26	ALA	3.6
1	D	251	GLY	3.6
1	D	268	ASP	3.6
1	D	190	SER	3.5
1	D	248	ARG	3.5
1	D	84	GLU	3.3
1	D	71	GLY	3.3
1	B	2	ALA	3.3
1	D	189	ILE	3.2
1	B	230[A]	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	94	THR	3.1
1	D	250	LEU	3.1
1	C	366	ARG	3.0
1	D	87	ARG	3.0
1	C	3	ALA	3.0
1	D	72	LEU	3.0
1	D	22	GLU	3.0
1	D	96	GLN	3.0
1	D	270	VAL	2.9
1	D	3	ALA	2.9
1	D	103	THR	2.9
1	D	70	ASP	2.9
1	D	34	ALA	2.9
1	D	387	ALA	2.9
1	D	93	PRO	2.9
1	C	241	ARG	2.8
1	D	192	MET	2.8
1	D	73	VAL	2.8
1	D	21	ARG	2.8
1	D	126	SER	2.7
1	D	25	GLY	2.7
1	D	191	LEU	2.7
1	D	143	ALA	2.7
1	C	230	SER	2.7
1	C	268	ASP	2.7
1	C	274	GLY	2.7
1	D	2	ALA	2.6
1	D	68	ARG	2.6
1	D	18	ARG	2.6
1	D	24	PHE	2.5
1	D	185	MET	2.5
1	D	80	GLU	2.5
1	B	232[A]	ALA	2.5
1	D	264	GLU	2.5
1	D	272	LYS	2.4
1	C	370	GLU	2.4
1	D	90	PHE	2.4
1	D	193	GLY	2.4
1	D	144	SER	2.4
1	B	228[A]	ARG	2.3
1	C	233	SER	2.3
1	D	122	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	125	PHE	2.3
1	C	365	MET	2.3
1	D	97	ARG	2.3
1	D	249	ALA	2.3
1	D	35	PRO	2.2
1	D	140	SER	2.2
1	C	249	ALA	2.2
1	C	264	GLU	2.2
1	D	5	ARG	2.2
1	C	265	ALA	2.2
1	D	119	ALA	2.2
1	D	267	ARG	2.2
1	D	101	PRO	2.1
1	C	245	GLU	2.1
1	B	359	SER	2.1
1	D	27	GLU	2.1
1	D	245	GLU	2.0
1	D	386	GLY	2.0
1	D	123	PRO	2.0

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 monosaccharides 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
5	MG	D	406	1/1	0.78	1.02	94,94,94,94	0
4	PO4	A	403	5/5	0.79	0.20	91,95,114,115	0
4	PO4	C	403	5/5	0.82	0.21	95,101,122,126	0
4	PO4	C	404	5/5	0.83	0.31	103,108,128,135	0

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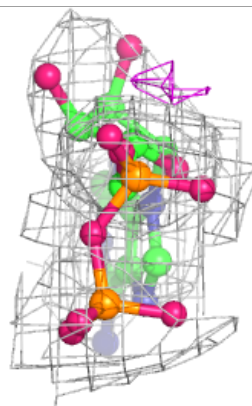
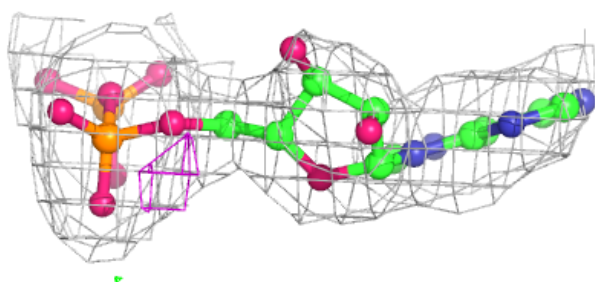
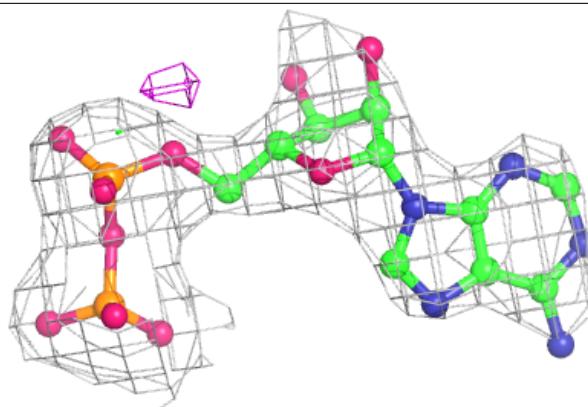
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PO4	B	404	5/5	0.83	0.18	97,107,121,123	0
4	PO4	A	405	5/5	0.84	0.23	81,89,116,116	0
5	MG	B	406	1/1	0.85	0.11	72,72,72,72	0
4	PO4	D	404	5/5	0.88	0.12	72,94,112,114	0
4	PO4	B	405	5/5	0.89	0.18	70,78,103,110	0
4	PO4	B	403	5/5	0.89	0.20	86,91,102,102	0
5	MG	C	405	1/1	0.91	0.16	96,96,96,96	0
4	PO4	D	403	5/5	0.91	0.24	88,92,96,110	0
4	PO4	A	404	5/5	0.92	0.11	74,82,90,96	0
4	PO4	D	405	5/5	0.93	0.22	98,106,121,129	0
3	ADP	D	402	27/27	0.94	0.17	64,83,90,92	0
6	NA	B	407	1/1	0.94	0.05	43,43,43,43	0
2	GLA	C	401	12/12	0.97	0.21	57,63,65,66	0
5	MG	A	406	1/1	0.97	0.13	60,60,60,60	0
2	GLA	B	401	12/12	0.97	0.13	41,43,46,47	0
6	NA	C	406	1/1	0.97	0.12	65,65,65,65	0
6	NA	A	407	1/1	0.98	0.05	37,37,37,37	0
2	GLA	A	401	12/12	0.98	0.13	39,43,46,46	0
3	ADP	C	402	27/27	0.98	0.12	47,53,58,61	0
6	NA	D	407	1/1	0.98	0.08	51,51,51,51	0
2	GLA	D	401	12/12	0.99	0.26	55,57,59,61	0
3	ADP	A	402	27/27	0.99	0.10	43,48,52,53	0
3	ADP	B	402	27/27	0.99	0.10	43,45,48,55	0

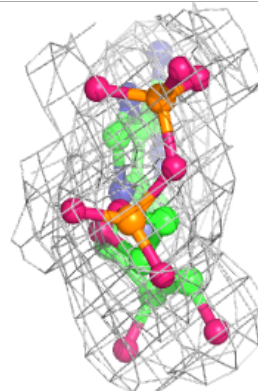
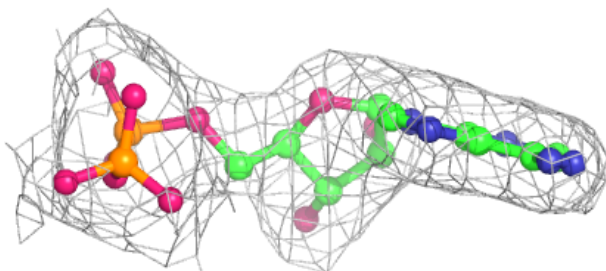
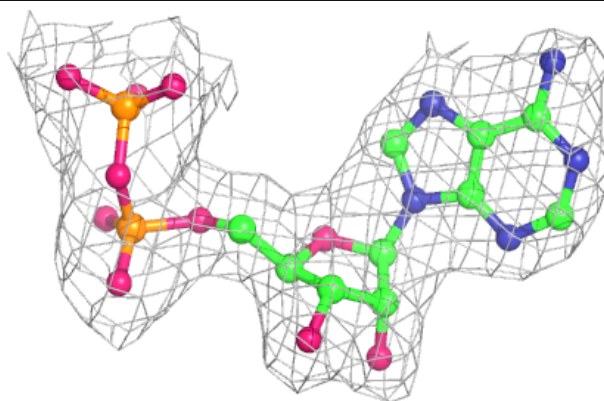
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 402:

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

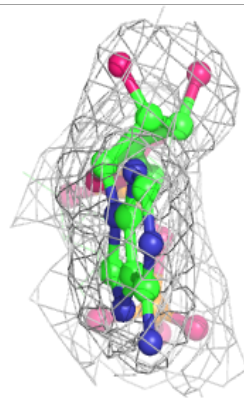
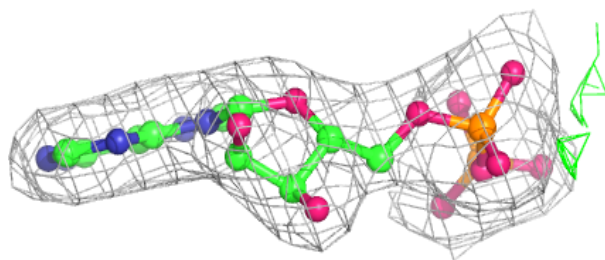
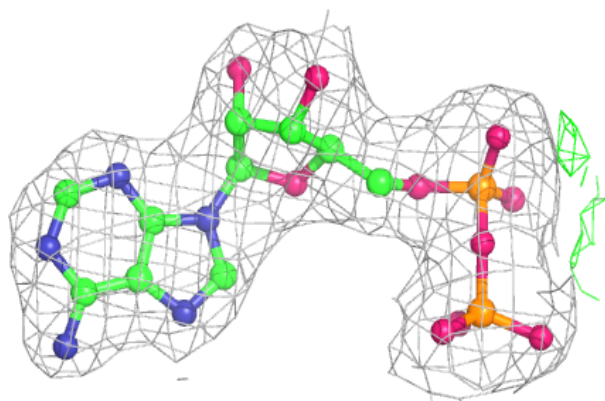
**Electron density around ADP C 402:**

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

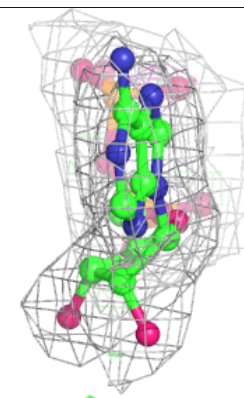
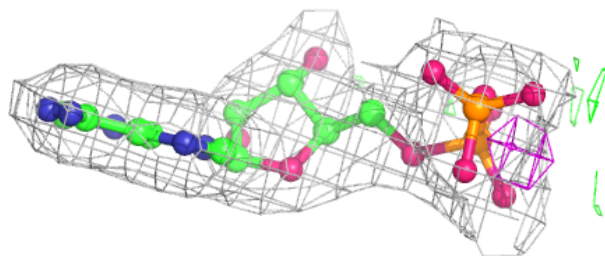
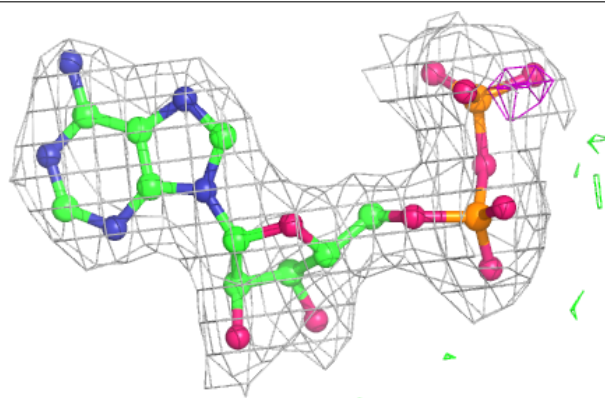


Electron density around ADP A 402:

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

**Electron density around ADP B 402:**

$2mF_o-DF_c$ (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.