



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:35 AM UTC

PDB ID : 1DGK / pdb_00001dgk
Title : MUTANT MONOMER OF RECOMBINANT HUMAN HEXOKINASE
TYPE I WITH GLUCOSE AND ADP IN THE ACTIVE SITE
Authors : Aleshin, A.E.; Liu, X.; Kirby, C.; Bourenkov, G.P.; Bartunik, H.D.; Fromm,
H.J.; Honzatko, R.B.
Deposited on : 1999-11-24
Resolution : 2.80 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

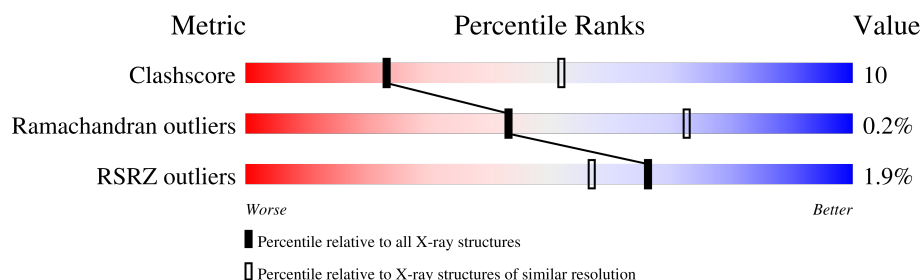
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	N	917	

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	ADP	N	921	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7256 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.

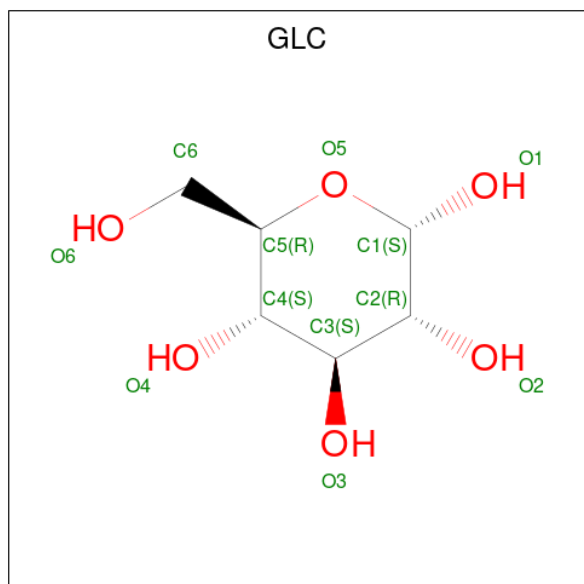
- Molecule 1 is a protein called HEXOKINASE TYPE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	N	898	7079	4435	1257	1333	54	0	13	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	240	GLU	ALA	engineered mutation	UNP P19367
N	243	ARG	ALA	engineered mutation	UNP P19367
N	284	TYR	GLY	engineered mutation	UNP P19367
N	536	ALA	THR	engineered mutation	UNP P19367
N	730	ASP	ASN	conflict	UNP P19367
N	776	LEU	MET	conflict	UNP P19367

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



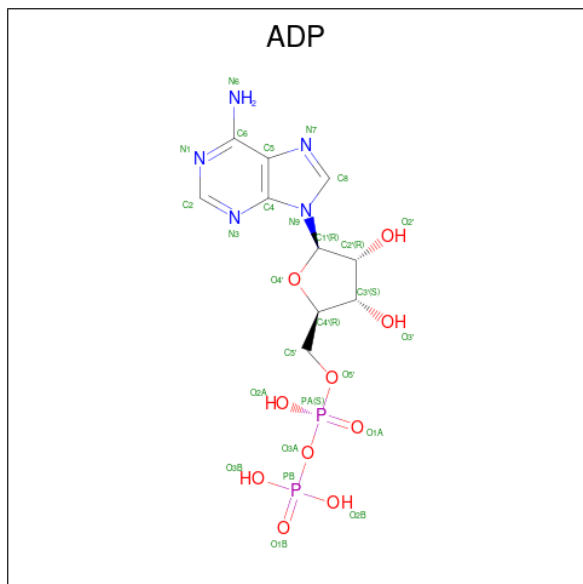
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	N	1	Total	C	O	0	0
			12	6	6		
2	N	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

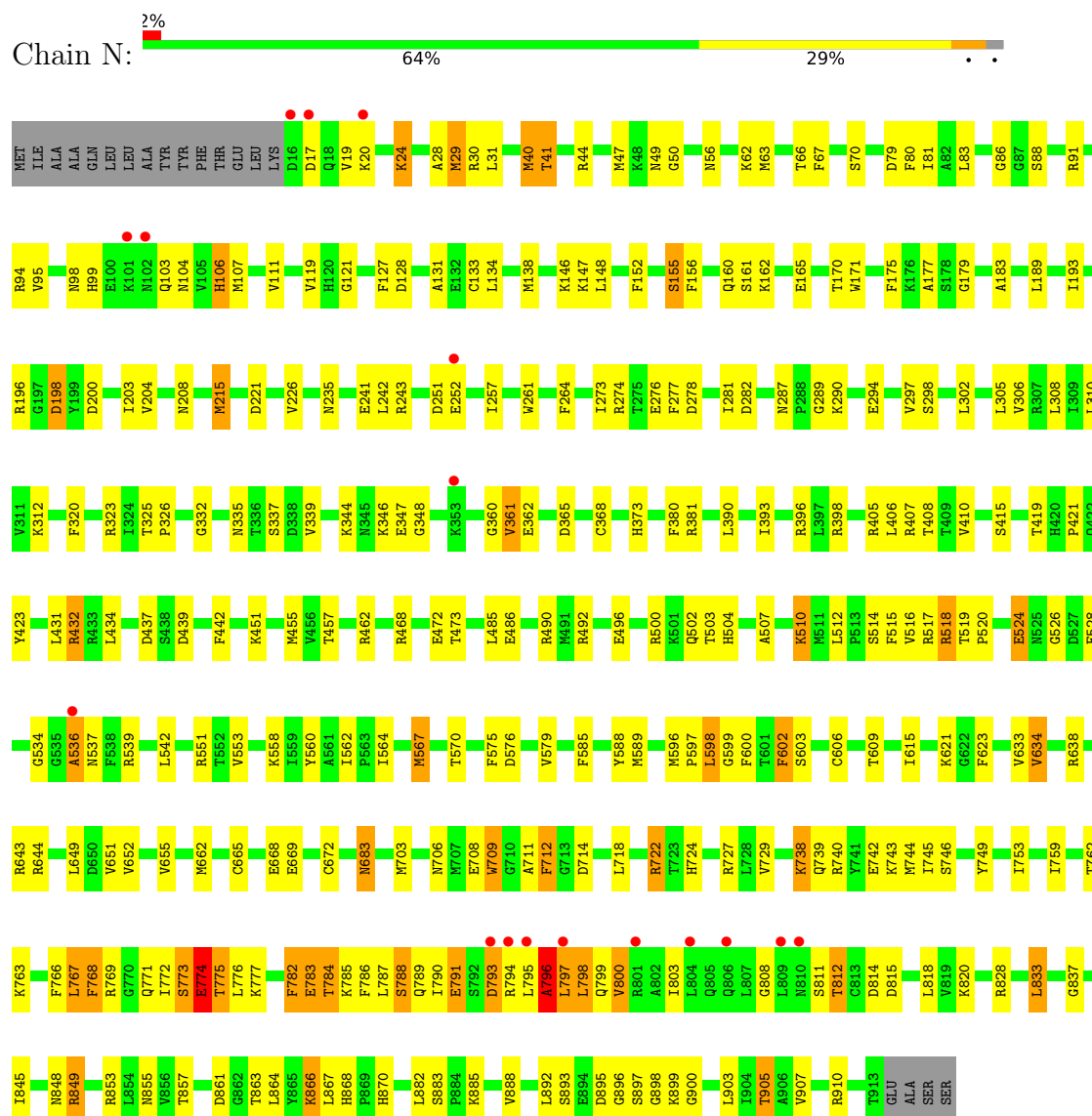
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	N	94	Total	O	0	0
			94	94		

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: HEXOKINASE TYPE I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.78Å 146.83Å 58.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	78.0 (8.00-2.80) 75.1 (8.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.258 , 0.308 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7256	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: ADP, GLC, PO4

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	N	0.68	0/7247	1.97	234/9750 (2.4%)

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	N	0	1

There are no bond length outliers.

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	N	722	ARG	NE-CZ-NH2	14.00	131.80	119.20
1	N	297	VAL	N-CA-C	12.76	122.54	111.56
1	N	264	PHE	CA-CB-CG	10.49	124.29	113.80
1	N	56	ASN	OD1-CG-ND2	10.43	133.03	122.60
1	N	17	ASP	CA-CB-CG	9.87	122.47	112.60
1	N	243	ARG	CD-NE-CZ	9.68	137.96	124.40
1	N	774	GLU	CA-C-O	-9.58	106.81	120.51
1	N	746	SER	N-CA-C	9.52	122.80	110.53
1	N	727	ARG	NE-CZ-NH2	9.51	127.76	119.20
1	N	712	PHE	CA-CB-CG	9.29	123.09	113.80
1	N	515	PHE	CA-CB-CG	-9.29	104.51	113.80
1	N	727	ARG	NE-CZ-NH1	-9.09	112.41	121.50
1	N	745	ILE	N-CA-C	8.91	119.22	111.56
1	N	812	THR	N-CA-C	-8.71	97.34	110.14
1	N	468	ARG	NE-CZ-NH1	-8.44	113.06	121.50
1	N	722	ARG	NH1-CZ-NH2	-8.19	108.66	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	796	ALA	N-CA-C	-8.14	102.79	112.89
1	N	798	LEU	N-CA-C	-7.99	102.80	112.54
1	N	782	PHE	CA-CB-CG	-7.93	105.87	113.80
1	N	468	ARG	NE-CZ-NH2	7.89	126.30	119.20
1	N	208	ASN	CA-C-O	-7.87	112.53	121.81
1	N	297	VAL	CB-CA-C	-7.70	104.12	111.44
1	N	746	SER	CA-C-N	7.70	128.65	120.03
1	N	746	SER	C-N-CA	7.70	128.65	120.03
1	N	855	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	N	795	LEU	N-CA-C	-7.63	104.46	114.31
1	N	40	MET	O-C-N	-7.54	114.30	122.07
1	N	492	ARG	NH1-CZ-NH2	7.53	129.09	119.30
1	N	837	GLY	N-CA-C	-7.53	103.38	112.49
1	N	745	ILE	CB-CA-C	-7.50	104.31	111.44
1	N	634	VAL	CA-C-O	7.44	128.74	120.85
1	N	408	THR	O-C-N	7.33	131.26	123.42
1	N	106	HIS	CA-C-O	-7.32	111.28	120.28
1	N	783	GLU	CA-C-N	-7.25	109.25	122.38
1	N	783	GLU	C-N-CA	-7.25	109.25	122.38
1	N	897	SER	CA-C-N	7.21	128.13	119.99
1	N	897	SER	C-N-CA	7.21	128.13	119.99
1	N	361	VAL	CA-C-N	7.10	131.74	123.15
1	N	361	VAL	C-N-CA	7.10	131.74	123.15
1	N	669	GLU	CA-C-O	7.05	126.08	119.59
1	N	900	GLY	O-C-N	-7.04	115.36	122.19
1	N	729	VAL	CA-C-O	-6.99	113.76	121.17
1	N	49	ASN	CA-C-N	6.98	127.69	119.94
1	N	49	ASN	C-N-CA	6.98	127.69	119.94
1	N	576	ASP	CB-CG-OD2	-6.96	102.39	118.40
1	N	274	ARG	O-C-N	-6.95	114.41	122.89
1	N	302	LEU	CA-C-O	-6.94	113.20	120.55
1	N	655	VAL	N-CA-CB	-6.92	100.09	111.44
1	N	512	LEU	N-CA-C	6.88	118.32	109.65
1	N	828	ARG	NH1-CZ-NH2	6.88	128.24	119.30
1	N	406	LEU	CA-C-O	-6.83	112.93	120.38
1	N	261	TRP	CA-CB-CG	6.79	126.50	113.60
1	N	179	GLY	CA-C-N	-6.77	116.09	122.66
1	N	179	GLY	C-N-CA	-6.77	116.09	122.66
1	N	308	LEU	CA-C-O	-6.72	113.42	120.55
1	N	380	PHE	CA-CB-CG	6.72	120.53	113.80
1	N	332	GLY	CA-C-O	6.69	126.14	119.04
1	N	361	VAL	CA-C-O	6.68	129.13	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	811	SER	O-C-N	6.67	130.45	122.85
1	N	861	ASP	CA-C-O	-6.63	114.21	121.31
1	N	504	HIS	CA-CB-CG	-6.61	107.19	113.80
1	N	600	PHE	CA-CB-CG	6.60	120.40	113.80
1	N	215	MET	CA-C-O	6.59	127.41	120.42
1	N	528	PHE	CA-C-O	-6.58	113.41	121.11
1	N	79	ASP	CA-CB-CG	6.55	119.15	112.60
1	N	242	LEU	CA-C-O	-6.54	113.62	120.55
1	N	298	SER	CA-C-N	6.52	128.29	120.14
1	N	298	SER	C-N-CA	6.52	128.29	120.14
1	N	67	PHE	CA-CB-CG	-6.51	107.29	113.80
1	N	290	LYS	CA-C-O	6.47	128.42	121.11
1	N	643	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	N	828	ARG	NE-CZ-NH2	-6.46	113.38	119.20
1	N	31	LEU	N-CA-C	6.45	119.60	110.50
1	N	473	THR	CA-CB-OG1	-6.42	99.98	109.60
1	N	797	LEU	N-CA-C	-6.42	103.43	111.90
1	N	706	ASN	CA-C-O	-6.41	114.26	120.92
1	N	542	LEU	CA-C-O	-6.38	113.47	120.30
1	N	337	SER	CA-C-O	6.35	127.28	120.55
1	N	360	GLY	N-CA-C	-6.32	105.79	114.64
1	N	784	THR	N-CA-C	-6.31	105.34	113.16
1	N	746	SER	CA-C-O	6.30	129.19	121.94
1	N	407	ARG	NE-CZ-NH2	6.26	124.84	119.20
1	N	870	HIS	CB-CG-CD2	6.26	139.34	131.20
1	N	148	LEU	O-C-N	6.26	126.63	121.31
1	N	347	GLU	CB-CG-CD	6.26	123.24	112.60
1	N	41	THR	CA-CB-CG2	6.25	121.13	110.50
1	N	278	ASP	CA-C-O	6.24	127.37	120.82
1	N	30	ARG	N-CA-CB	-6.24	101.32	110.49
1	N	251	ASP	CA-C-N	6.23	131.28	121.99
1	N	251	ASP	C-N-CA	6.23	131.28	121.99
1	N	709	TRP	CA-CB-CG	6.23	125.44	113.60
1	N	562	ILE	N-CA-CB	6.20	117.75	111.36
1	N	510	LYS	N-CA-C	6.18	118.82	111.71
1	N	127	PHE	CA-CB-CG	-6.17	107.63	113.80
1	N	576	ASP	CA-C-O	6.11	127.03	120.55
1	N	390	LEU	O-C-N	-6.10	115.66	122.12
1	N	539	ARG	NE-CZ-NH2	-6.09	113.71	119.20
1	N	80	PHE	N-CA-C	6.08	119.46	109.85
1	N	712	PHE	CA-C-O	-6.08	114.46	121.15
1	N	415	SER	CA-CB-OG	-6.06	98.98	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	252	GLU	N-CA-C	6.05	118.05	108.67
1	N	524	GLU	CB-CG-CD	6.04	122.87	112.60
1	N	798	LEU	CA-C-N	6.04	128.65	120.44
1	N	798	LEU	C-N-CA	6.04	128.65	120.44
1	N	898	GLY	N-CA-C	6.01	119.91	112.64
1	N	517	ARG	CG-CD-NE	5.99	125.17	112.00
1	N	200	ASP	CA-CB-CG	5.97	118.57	112.60
1	N	738	LYS	CA-C-O	-5.96	114.48	121.46
1	N	745	ILE	N-CA-CB	-5.94	104.88	111.41
1	N	40	MET	CA-C-N	5.92	128.69	120.29
1	N	40	MET	C-N-CA	5.92	128.69	120.29
1	N	567	MET	CA-C-O	5.91	126.77	119.97
1	N	708	GLU	N-CA-C	-5.91	103.25	111.52
1	N	99	HIS	CA-C-O	5.89	126.19	119.18
1	N	492	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	N	771	GLN	N-CA-C	5.88	118.34	107.99
1	N	775	THR	CB-CA-C	5.88	122.27	109.99
1	N	381	ARG	NE-CZ-NH2	5.87	124.49	119.20
1	N	510	LYS	CA-C-O	-5.86	113.47	120.10
1	N	472	GLU	CA-C-O	-5.85	114.64	120.90
1	N	576	ASP	CB-CG-OD1	5.85	131.85	118.40
1	N	24	LYS	N-CA-C	-5.84	104.83	111.14
1	N	432	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	N	49	ASN	CA-C-O	5.82	126.71	120.55
1	N	83	LEU	CA-C-O	-5.80	114.44	121.28
1	N	155	SER	N-CA-C	5.79	118.60	109.39
1	N	235	ASN	CA-CB-CG	5.79	118.39	112.60
1	N	744	MET	O-C-N	5.79	130.01	122.42
1	N	724	HIS	O-C-N	-5.79	115.45	122.22
1	N	800	VAL	CA-C-N	5.79	128.31	120.44
1	N	800	VAL	C-N-CA	5.79	128.31	120.44
1	N	905	THR	CA-CB-CG2	-5.78	100.67	110.50
1	N	738	LYS	N-CA-CB	-5.78	101.84	111.20
1	N	683	ASN	CA-CB-CG	5.77	118.37	112.60
1	N	849	ARG	CA-C-O	5.76	126.40	119.43
1	N	793	ASP	CA-CB-CG	-5.76	106.84	112.60
1	N	615	ILE	CB-CG1-CD1	5.75	125.88	113.80
1	N	855	ASN	CB-CG-ND2	5.74	125.01	116.40
1	N	50	GLY	O-C-N	5.74	127.69	122.18
1	N	419	THR	N-CA-C	5.74	120.55	113.50
1	N	588	TYR	CA-C-O	-5.72	114.49	120.55
1	N	348	GLY	O-C-N	-5.70	115.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	893	SER	CA-CB-OG	-5.68	99.73	111.10
1	N	410	VAL	CA-C-O	-5.68	114.45	120.53
1	N	88	SER	CA-C-O	-5.67	113.45	119.97
1	N	744	MET	CA-C-O	-5.66	112.70	119.15
1	N	848	ASN	CB-CG-ND2	5.66	124.88	116.40
1	N	575	PHE	CA-CB-CG	-5.65	108.15	113.80
1	N	784	THR	CB-CA-C	5.65	120.17	110.01
1	N	888	VAL	N-CA-C	5.64	116.22	107.99
1	N	297	VAL	N-CA-CB	-5.63	105.22	111.41
1	N	791	GLU	CA-C-O	5.63	126.49	119.12
1	N	599	GLY	O-C-N	5.62	128.97	123.80
1	N	517	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	N	564	ILE	O-C-N	-5.60	116.21	121.87
1	N	198	ASP	N-CA-C	5.60	119.28	112.23
1	N	602	PHE	CA-CB-CG	5.60	119.40	113.80
1	N	739	GLN	OE1-CD-NE2	5.57	128.17	122.60
1	N	749	TYR	N-CA-C	5.56	120.72	113.88
1	N	870	HIS	CB-CG-ND1	-5.53	114.41	122.70
1	N	598	LEU	CA-C-N	-5.52	117.60	122.73
1	N	598	LEU	C-N-CA	-5.52	117.60	122.73
1	N	423	TYR	N-CA-C	5.50	117.74	111.02
1	N	152	PHE	CA-CB-CG	5.50	119.30	113.80
1	N	599	GLY	CA-C-O	-5.49	115.59	120.75
1	N	221	ASP	CA-CB-CG	5.48	118.08	112.60
1	N	833	LEU	CA-C-O	5.47	126.33	120.70
1	N	298	SER	N-CA-C	5.46	117.92	110.55
1	N	895	ASP	N-CA-C	5.45	119.93	113.28
1	N	507	ALA	CA-C-O	-5.45	114.48	120.69
1	N	516	VAL	CA-C-O	-5.44	114.43	120.74
1	N	609	THR	N-CA-C	-5.43	106.66	113.72
1	N	518	ARG	CD-NE-CZ	5.42	131.99	124.40
1	N	621	LYS	CA-C-O	-5.42	111.73	119.80
1	N	703	MET	N-CA-CB	5.39	119.66	110.71
1	N	861	ASP	O-C-N	5.39	128.76	122.99
1	N	602	PHE	CA-C-O	-5.39	114.51	120.33
1	N	29	MET	CA-C-O	5.39	125.59	119.18
1	N	94	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	N	537	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	N	28	ALA	N-CA-C	5.38	119.47	113.01
1	N	287	ASN	CB-CG-ND2	-5.38	108.34	116.40
1	N	273	ILE	CA-CB-CG2	5.36	119.61	110.50
1	N	662	MET	O-C-N	-5.36	116.55	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	537	ASN	CA-CB-CG	-5.35	107.25	112.60
1	N	183	ALA	CA-C-O	-5.34	115.12	121.16
1	N	537	ASN	CB-CG-OD1	-5.33	110.15	120.80
1	N	226	VAL	CA-C-O	-5.32	115.11	121.28
1	N	514	SER	CA-CB-OG	-5.31	100.48	111.10
1	N	857	THR	CA-CB-OG1	-5.31	101.64	109.60
1	N	799	GLN	O-C-N	5.31	127.82	122.09
1	N	257	ILE	O-C-N	-5.29	117.63	123.18
1	N	669	GLU	CB-CA-C	-5.27	104.32	110.17
1	N	767	LEU	CB-CA-C	-5.26	97.88	109.56
1	N	302	LEU	O-C-N	5.26	127.69	122.12
1	N	791	GLU	N-CA-C	5.26	119.56	113.20
1	N	298	SER	CA-C-O	5.25	128.00	121.81
1	N	526	GLY	CA-C-O	-5.25	116.40	121.86
1	N	883	SER	CA-C-N	5.25	124.91	119.56
1	N	883	SER	C-N-CA	5.25	124.91	119.56
1	N	156	PHE	O-C-N	-5.25	118.18	121.85
1	N	133	CYS	N-CA-CB	5.24	117.91	110.16
1	N	742	GLU	CG-CD-OE2	5.24	130.45	118.40
1	N	794	ARG	N-CA-C	-5.23	101.84	109.63
1	N	56	ASN	CB-CG-OD1	-5.22	110.36	120.80
1	N	866	LYS	CA-C-O	-5.21	115.33	120.70
1	N	462	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	N	30	ARG	O-C-N	-5.19	116.68	122.55
1	N	346	LYS	CA-CB-CG	5.19	124.48	114.10
1	N	361	VAL	N-CA-CB	5.19	119.79	111.23
1	N	848	ASN	CB-CG-OD1	-5.18	110.44	120.80
1	N	128	ASP	N-CA-C	-5.18	105.71	111.36
1	N	662	MET	CA-C-O	5.17	126.25	120.82
1	N	215	MET	O-C-N	-5.15	116.28	122.15
1	N	655	VAL	N-CA-C	5.15	116.14	108.46
1	N	753	ILE	N-CA-C	-5.15	105.69	110.53
1	N	251	ASP	CA-C-O	5.14	125.55	119.48
1	N	241	GLU	O-C-N	-5.12	117.05	123.04
1	N	455	MET	CA-C-N	5.12	127.00	120.56
1	N	455	MET	C-N-CA	5.12	127.00	120.56
1	N	606	CYS	CA-C-O	-5.12	114.78	120.66
1	N	773	SER	O-C-N	5.12	129.22	122.93
1	N	855	ASN	N-CA-C	-5.11	98.94	107.99
1	N	66	THR	CA-C-O	5.08	124.64	119.05
1	N	896	GLY	N-CA-C	-5.08	104.19	112.83
1	N	528	PHE	CA-CB-CG	-5.07	108.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	131	ALA	CA-C-O	5.05	125.91	120.55
1	N	339	VAL	O-C-N	5.04	126.85	121.91
1	N	297	VAL	CA-C-O	-5.04	115.89	120.73
1	N	768	PHE	N-CA-C	5.04	118.55	111.90
1	N	788	SER	CA-C-O	5.03	125.83	120.24
1	N	510	LYS	CD-CE-NZ	5.03	127.99	111.90
1	N	536	ALA	N-CA-CB	5.02	117.34	110.07
1	N	766	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	796	ALA	Mainchain

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	N	7079	0	7138	146	0
2	N	24	0	22	1	0
3	N	5	0	0	0	0
4	N	54	0	23	14	0
5	N	94	0	0	3	0
All	All	7256	0	7183	146	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 10.

All (146) 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:N:196[A]:ARG:HG2	1:N:198:ASP:HB2	1.31	1.13
1:N:361:VAL:HG12	1:N:362:GLU:H	1.36	0.90
1:N:323[A]:ARG:HD3	1:N:361:VAL:HG13	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:553:VAL:HG11	1:N:899:LYS:HG3	1.62	0.81
1:N:536:ALA:HB3	4:N:921:ADP:O2B	1.83	0.78
1:N:772:ILE:HG22	1:N:777:LYS:HG3	1.64	0.78
1:N:103:GLN:HE21	1:N:106:HIS:HB2	1.47	0.78
1:N:867:LEU:HD12	4:N:921:ADP:C5	2.19	0.77
1:N:95:VAL:HG22	1:N:107:MET:HE2	1.67	0.77
1:N:524:GLU:HA	1:N:910:ARG:HH22	1.49	0.77
1:N:867:LEU:HD12	4:N:921:ADP:C6	2.21	0.76
1:N:320:PHE:HB3	1:N:361:VAL:HG11	1.66	0.75
1:N:784:THR:HA	1:N:787:LEU:HB2	1.68	0.75
1:N:789:GLN:HB3	1:N:803:ILE:HD11	1.69	0.75
1:N:863:THR:HB	4:N:921:ADP:O4'	1.88	0.73
1:N:41:THR:HG23	1:N:44[B]:ARG:HH21	1.54	0.73
1:N:431:LEU:HD22	1:N:442:PHE:HZ	1.56	0.71
1:N:323[A]:ARG:CD	1:N:361:VAL:HG13	2.23	0.69
1:N:40:MET:HE1	1:N:434:LEU:HB3	1.76	0.68
1:N:788:SER:HB2	4:N:921:ADP:HN62	1.57	0.68
1:N:718:LEU:O	1:N:722:ARG:HG3	1.94	0.68
1:N:323[B]:ARG:NH1	1:N:362:GLU:HB2	2.09	0.68
1:N:325:THR:HB	1:N:326:PRO:HD2	1.79	0.64
1:N:812:THR:H	1:N:815:ASP:HB2	1.63	0.63
1:N:107:MET:HE1	1:N:451:LYS:HB2	1.80	0.62
1:N:119:VAL:HG13	1:N:175:PHE:HA	1.81	0.61
1:N:773:SER:O	1:N:774:GLU:C	2.39	0.61
1:N:162:LYS:HG2	1:N:165[A]:GLU:HG2	1.81	0.61
1:N:519:THR:HB	1:N:520:PRO:HD2	1.84	0.59
1:N:866:LYS:HG2	1:N:892:LEU:HD21	1.85	0.59
1:N:536:ALA:HB3	4:N:921:ADP:PB	2.42	0.58
1:N:570:THR:HB	5:N:973:HOH:O	2.01	0.58
1:N:598:LEU:C	1:N:598:LEU:HD23	2.29	0.58
1:N:134:LEU:HD11	1:N:138:MET:HE3	1.86	0.58
1:N:323[B]:ARG:HH12	1:N:362:GLU:HB2	1.68	0.57
1:N:767:LEU:HG	1:N:818:LEU:HD23	1.86	0.57
1:N:773:SER:O	1:N:775:THR:N	2.38	0.56
1:N:783:GLU:HB2	1:N:786:PHE:HD2	1.71	0.56
1:N:486:GLU:O	1:N:490:ARG:HG3	2.04	0.56
1:N:793:ASP:OD1	1:N:820:LYS:HE3	2.06	0.56
1:N:161:SER:N	1:N:165[A]:GLU:OE1	2.36	0.56
1:N:790:ILE:HG13	1:N:803:ILE:HD13	1.87	0.55
1:N:170[B]:THR:HG22	1:N:171:TRP:O	2.06	0.54
1:N:785:LYS:HA	4:N:921:ADP:C5	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:81:ILE:HD12	1:N:138:MET:HE2	1.90	0.53
1:N:759:ILE:HG22	1:N:763:LYS:HE3	1.90	0.53
1:N:773:SER:O	1:N:776:LEU:N	2.39	0.53
1:N:281:ILE:HG21	1:N:305:LEU:HD21	1.91	0.53
1:N:788:SER:OG	1:N:868:HIS:HA	2.10	0.52
1:N:189:LEU:HD23	1:N:203:ILE:HD13	1.91	0.52
1:N:551:ARG:HH21	1:N:668:GLU:CD	2.18	0.52
1:N:344:LYS:HG2	1:N:421:PRO:HG3	1.91	0.51
1:N:596:MET:HB3	1:N:597:PRO:HD2	1.92	0.51
1:N:524:GLU:HA	1:N:910:ARG:NH2	2.20	0.51
1:N:853:ARG:HA	1:N:885:LYS:O	2.10	0.51
1:N:634:VAL:O	1:N:638:ARG:HG3	2.10	0.51
1:N:496:GLU:OE2	1:N:500:ARG:NH1	2.43	0.51
1:N:19:VAL:HG13	1:N:373:HIS:CE1	2.46	0.51
1:N:81:ILE:CD1	1:N:138:MET:HE2	2.40	0.50
1:N:665:CYS:SG	1:N:672:CYS:SG	3.06	0.50
1:N:294:GLU:OE2	2:N:918:GLC:O1	2.30	0.50
1:N:759:ILE:HG23	1:N:772:ILE:HD12	1.94	0.50
1:N:785:LYS:HA	4:N:921:ADP:N7	2.28	0.49
1:N:767:LEU:CD2	1:N:818:LEU:HD23	2.43	0.49
1:N:103:GLN:NE2	1:N:106:HIS:HB2	2.20	0.49
1:N:518:ARG:NH2	1:N:907:VAL:HG22	2.27	0.49
1:N:510:LYS:NZ	5:N:995:HOH:O	2.46	0.49
1:N:20:LYS:O	1:N:24:LYS:HG3	2.13	0.48
1:N:845:ILE:O	1:N:849:ARG:HG3	2.12	0.48
1:N:431:LEU:HD22	1:N:442:PHE:CZ	2.44	0.48
1:N:782:PHE:O	1:N:783:GLU:C	2.56	0.48
1:N:867:LEU:HD12	4:N:921:ADP:N7	2.29	0.48
1:N:62:LYS:O	1:N:63:MET:C	2.56	0.47
1:N:107:MET:CE	1:N:451:LYS:HB2	2.44	0.47
1:N:95:VAL:CG2	1:N:107:MET:HE2	2.39	0.47
1:N:683:ASN:HA	1:N:709:TRP:CD1	2.49	0.47
1:N:768:PHE:O	1:N:769:ARG:HB2	2.14	0.47
1:N:812:THR:HG22	1:N:814:ASP:H	1.79	0.47
1:N:44[A]:ARG:HH11	1:N:44[A]:ARG:HG2	1.79	0.47
1:N:519:THR:HB	1:N:520:PRO:CD	2.45	0.47
1:N:524:GLU:HA	1:N:910:ARG:HH12	1.79	0.47
1:N:711:ALA:O	1:N:712:PHE:C	2.58	0.47
1:N:864:LEU:HD12	4:N:921:ADP:H2	1.80	0.46
1:N:161:SER:H	1:N:165[A]:GLU:CD	2.23	0.46
1:N:796:ALA:O	1:N:797:LEU:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:204:VAL:CG2	1:N:457:THR:HG23	2.46	0.46
1:N:344:LYS:HE3	1:N:421:PRO:HB3	1.97	0.46
1:N:714:ASP:OD1	1:N:740:ARG:HG3	2.16	0.46
1:N:649:LEU:HD23	1:N:649:LEU:HA	1.83	0.45
1:N:867:LEU:HD12	4:N:921:ADP:N6	2.31	0.45
1:N:398:ARG:NH2	1:N:437:ASP:HB2	2.32	0.45
1:N:405[A]:ARG:NH1	1:N:439:ASP:OD1	2.49	0.45
1:N:774:GLU:HA	1:N:774:GLU:OE1	2.17	0.45
1:N:432:ARG:HD2	5:N:939:HOH:O	2.14	0.45
1:N:567:MET:HE3	1:N:623:PHE:CE1	2.52	0.45
1:N:70:SER:O	1:N:215:MET:HE1	2.17	0.45
1:N:793:ASP:OD1	1:N:793:ASP:N	2.48	0.45
1:N:791:GLU:OE2	1:N:868:HIS:NE2	2.45	0.45
1:N:47:MET:HE1	1:N:393:ILE:HA	1.98	0.44
1:N:47:MET:HE2	1:N:396:ARG:HD3	1.99	0.44
1:N:585:PHE:CZ	1:N:589:MET:HG3	2.52	0.44
1:N:864:LEU:HA	4:N:921:ADP:N3	2.32	0.44
1:N:520:PRO:HG3	1:N:903:LEU:HD13	1.99	0.44
1:N:652:VAL:HB	1:N:905:THR:HG23	1.99	0.44
1:N:665:CYS:HG	1:N:672:CYS:CB	2.29	0.44
1:N:193:ILE:O	1:N:196[B]:ARG:HB2	2.18	0.44
1:N:866:LYS:HE3	1:N:892:LEU:HD11	2.00	0.44
1:N:19:VAL:HG13	1:N:373:HIS:NE2	2.32	0.44
1:N:306:VAL:O	1:N:310:LEU:HG	2.18	0.43
1:N:772:ILE:CG2	1:N:777:LYS:HG3	2.44	0.43
1:N:398:ARG:HH21	1:N:437:ASP:HB2	1.84	0.43
1:N:767:LEU:HD21	1:N:818:LEU:HB3	2.01	0.43
1:N:790:ILE:HG23	1:N:800:VAL:HG22	2.00	0.43
1:N:29:MET:HE3	1:N:277:PHE:HD2	1.84	0.43
1:N:121:GLY:O	1:N:177:ALA:HA	2.18	0.43
1:N:864:LEU:HA	4:N:921:ADP:C2	2.54	0.42
1:N:365:ASP:O	1:N:368:CYS:HB2	2.19	0.42
1:N:762:THR:HB	1:N:772:ILE:HD13	2.01	0.42
1:N:485:LEU:HD23	1:N:882:LEU:HD22	2.00	0.42
1:N:579:VAL:HG12	1:N:644:ARG:HD2	2.01	0.42
1:N:789:GLN:HB3	1:N:803:ILE:CD1	2.45	0.42
1:N:796:ALA:C	1:N:798:LEU:N	2.74	0.42
1:N:189:LEU:HD23	1:N:203:ILE:CD1	2.50	0.42
1:N:788:SER:OG	4:N:921:ADP:N1	2.39	0.42
1:N:98:ASN:ND2	1:N:104:ASN:HA	2.35	0.42
1:N:91:ARG:HG2	1:N:111:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:431:LEU:O	1:N:431:LEU:HG	2.16	0.41
1:N:634:VAL:HG13	1:N:651:VAL:HG11	2.02	0.41
1:N:553:VAL:HG21	1:N:899:LYS:HD3	2.02	0.41
1:N:276:GLU:OE1	1:N:312:LYS:HE3	2.21	0.41
1:N:282:ASP:CG	1:N:289:GLY:H	2.29	0.41
1:N:602:PHE:CE1	1:N:633:VAL:HG11	2.54	0.41
1:N:518:ARG:HH22	1:N:907:VAL:HG22	1.86	0.41
1:N:534:GLY:HA3	1:N:603:SER:OG	2.20	0.41
1:N:558:LYS:HE2	1:N:560:TYR:CE2	2.56	0.41
1:N:738:LYS:O	1:N:743:LYS:NZ	2.31	0.40
1:N:146:LYS:O	1:N:147:LYS:HB2	2.21	0.40
1:N:323[A]:ARG:HD3	1:N:361:VAL:HA	2.03	0.40
1:N:796:ALA:O	1:N:798:LEU:N	2.54	0.40
1:N:598:LEU:HD13	1:N:649:LEU:HD13	2.02	0.40
1:N:119:VAL:CG1	1:N:175:PHE:HA	2.49	0.40
1:N:502:GLN:HG2	1:N:503:THR:HG23	2.04	0.40
1:N:833:LEU:HD23	1:N:833:LEU:HA	1.93	0.40
1:N:86:GLY:HA3	1:N:155:SER:OG	2.21	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	N	909/917 (99%)	878 (97%)	29 (3%)	2 (0%)	43 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	774	GLU
1	N	808	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	N	919	-	12,12,12	0.52	0	17,17,17	2.15	6 (35%)
4	ADP	N	921	-	28,29,29	1.19	3 (10%)	43,45,45	1.55	11 (25%)
3	PO4	N	920	-	4,4,4	1.94	2 (50%)	6,6,6	1.91	1 (16%)
4	ADP	N	922	-	28,29,29	1.30	3 (10%)	43,45,45	1.51	7 (16%)
2	GLC	N	918	-	12,12,12	0.79	1 (8%)	17,17,17	1.84	4 (23%)

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	GLC	N	918	-	-	0/2/22/22	0/1/1/1
4	ADP	N	921	-	-	4/16/32/32	0/3/3/3
2	GLC	N	919	-	-	0/2/22/22	0/1/1/1
4	ADP	N	922	-	-	3/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	922	ADP	C5-N7	-3.99	1.31	1.39
4	N	921	ADP	C5-N7	-3.73	1.32	1.39
3	N	920	PO4	P-O3	-2.29	1.48	1.54
4	N	922	ADP	C2-N1	2.28	1.38	1.33
4	N	921	ADP	C2-N1	2.23	1.37	1.33
3	N	920	PO4	P-O4	2.23	1.61	1.54
4	N	921	ADP	PA-O2A	-2.13	1.45	1.55
2	N	918	GLC	O1-C1	-2.04	1.33	1.39
4	N	922	ADP	PB-O3B	-2.00	1.47	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	919	GLC	O2-C2-C3	-5.77	96.78	110.38
2	N	918	GLC	O3-C3-C2	-4.16	100.58	110.38
4	N	922	ADP	O2A-PA-O5'	4.03	125.82	107.57
3	N	920	PO4	O3-P-O2	-3.73	96.31	107.91
2	N	918	GLC	O1-C1-C2	3.60	119.44	108.98
4	N	921	ADP	O4'-C4'-C5'	3.56	120.74	109.33
4	N	922	ADP	C4-N9-C8	-3.28	102.29	105.74
4	N	921	ADP	O2A-PA-O3A	3.27	116.12	107.27
4	N	922	ADP	N9-C8-N7	3.13	118.38	113.94
4	N	922	ADP	C4-C5-N7	3.03	114.05	110.58
2	N	918	GLC	O5-C5-C6	-2.86	99.34	106.44
4	N	922	ADP	N3-C2-N1	-2.79	124.36	128.58
2	N	918	GLC	O6-C6-C5	2.77	120.75	111.33
2	N	919	GLC	C1-O5-C5	-2.74	108.34	113.65
4	N	921	ADP	C4-N9-C8	-2.74	102.86	105.74
4	N	921	ADP	O2B-PB-O3A	2.73	113.78	104.64
2	N	919	GLC	O4-C4-C5	-2.69	102.70	109.32
4	N	921	ADP	O5'-C5'-C4'	2.68	118.13	108.99
4	N	921	ADP	O3B-PB-O3A	2.59	113.32	104.64
2	N	919	GLC	O2-C2-C1	2.43	114.86	109.25
4	N	922	ADP	O3B-PB-O3A	2.41	112.71	104.64
4	N	921	ADP	O2A-PA-O1A	-2.40	101.29	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	922	ADP	C2'-C1'-N9	2.37	119.20	113.30
4	N	921	ADP	C6-C5-N7	-2.23	127.79	132.09
2	N	919	GLC	O3-C3-C2	-2.14	105.34	110.38
4	N	921	ADP	O2B-PB-O1B	-2.08	102.75	110.83
4	N	921	ADP	C2-N3-C4	-2.06	106.80	111.83
4	N	921	ADP	C6-C5-C4	2.03	119.94	117.18
2	N	919	GLC	O1-C1-O5	2.02	116.42	110.41

There are no chirality outliers.

All (7) torsion outliers are listed below:

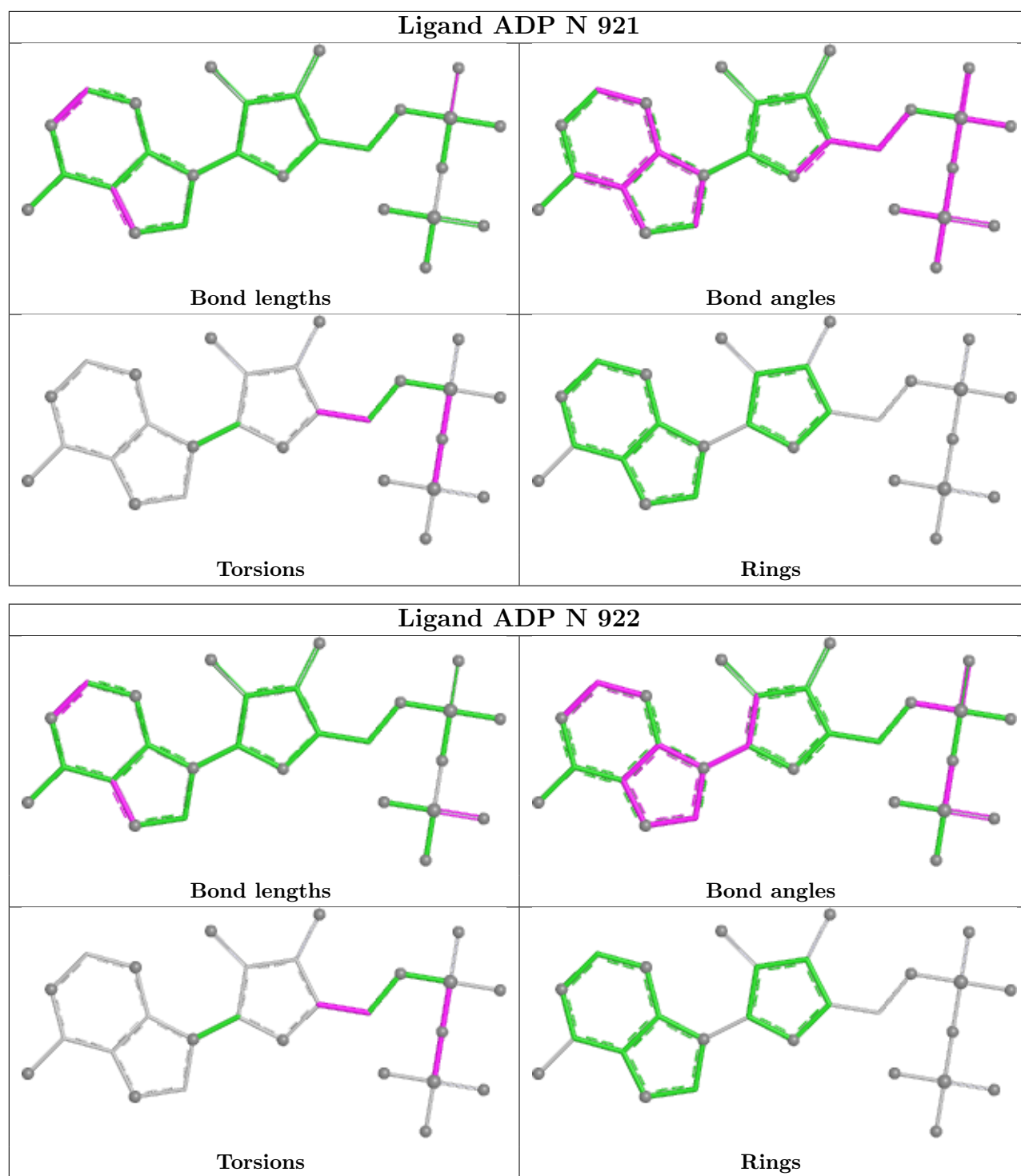
Mol	Chain	Res	Type	Atoms
4	N	922	ADP	C3'-C4'-C5'-O5'
4	N	922	ADP	PB-O3A-PA-O5'
4	N	921	ADP	PA-O3A-PB-O1B
4	N	921	ADP	C3'-C4'-C5'-O5'
4	N	921	ADP	PB-O3A-PA-O1A
4	N	921	ADP	PA-O3A-PB-O3B
4	N	922	ADP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	921	ADP	14	0
2	N	918	GLC	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	N	898/917 (97%)	-0.45	17 (1%) 66 57	27, 45, 77, 116	34 (3%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	102	ASN	5.1
1	N	17	ASP	4.5
1	N	20	LYS	4.1
1	N	809	LEU	3.5
1	N	16	ASP	3.5
1	N	252	GLU	3.4
1	N	101	LYS	3.3
1	N	806	GLN	3.1
1	N	793	ASP	3.1
1	N	794	ARG	3.1
1	N	797	LEU	2.9
1	N	804	LEU	2.7
1	N	810	ASN	2.7
1	N	801	ARG	2.6
1	N	353	LYS	2.3
1	N	536	ALA	2.2
1	N	795	LEU	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](#)

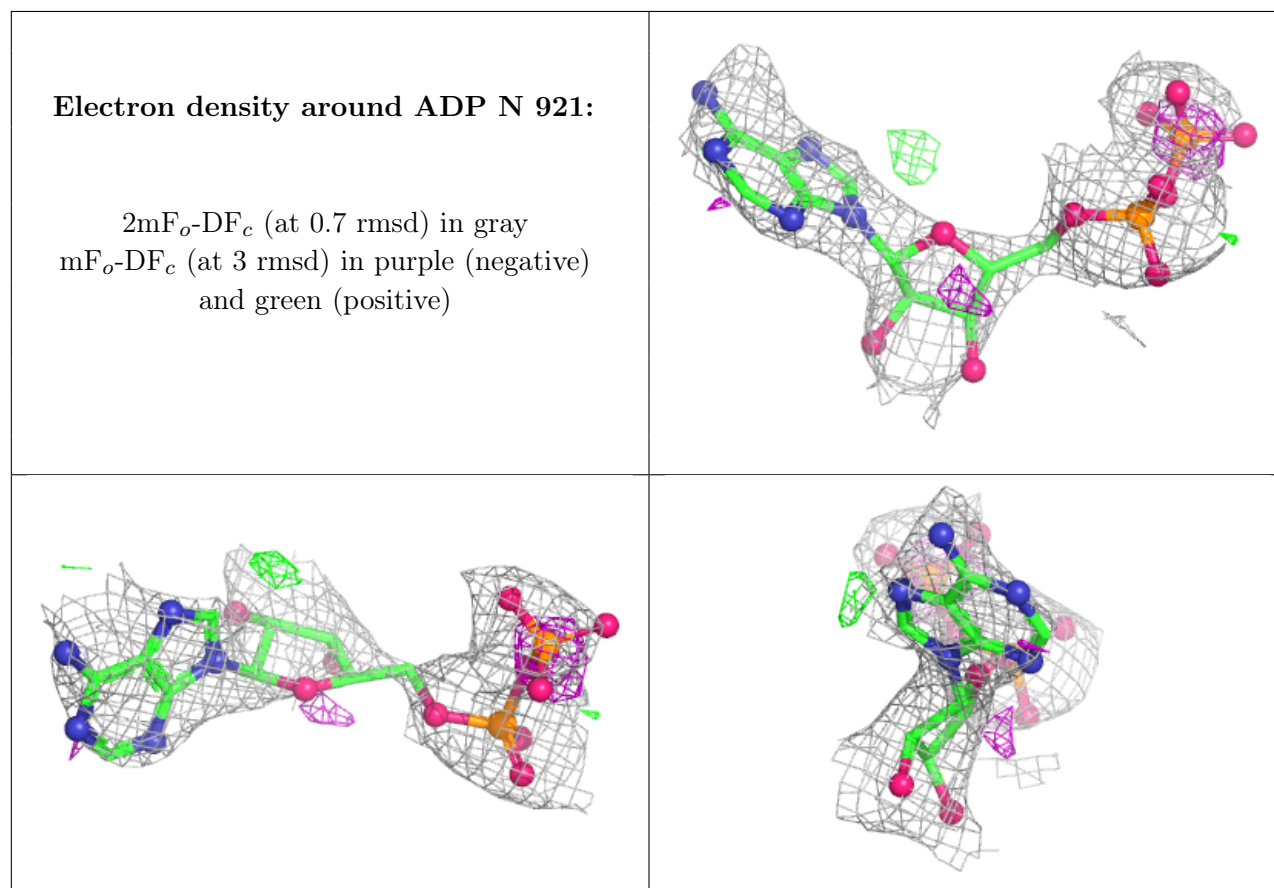
There are no oligosaccharides in this entry.

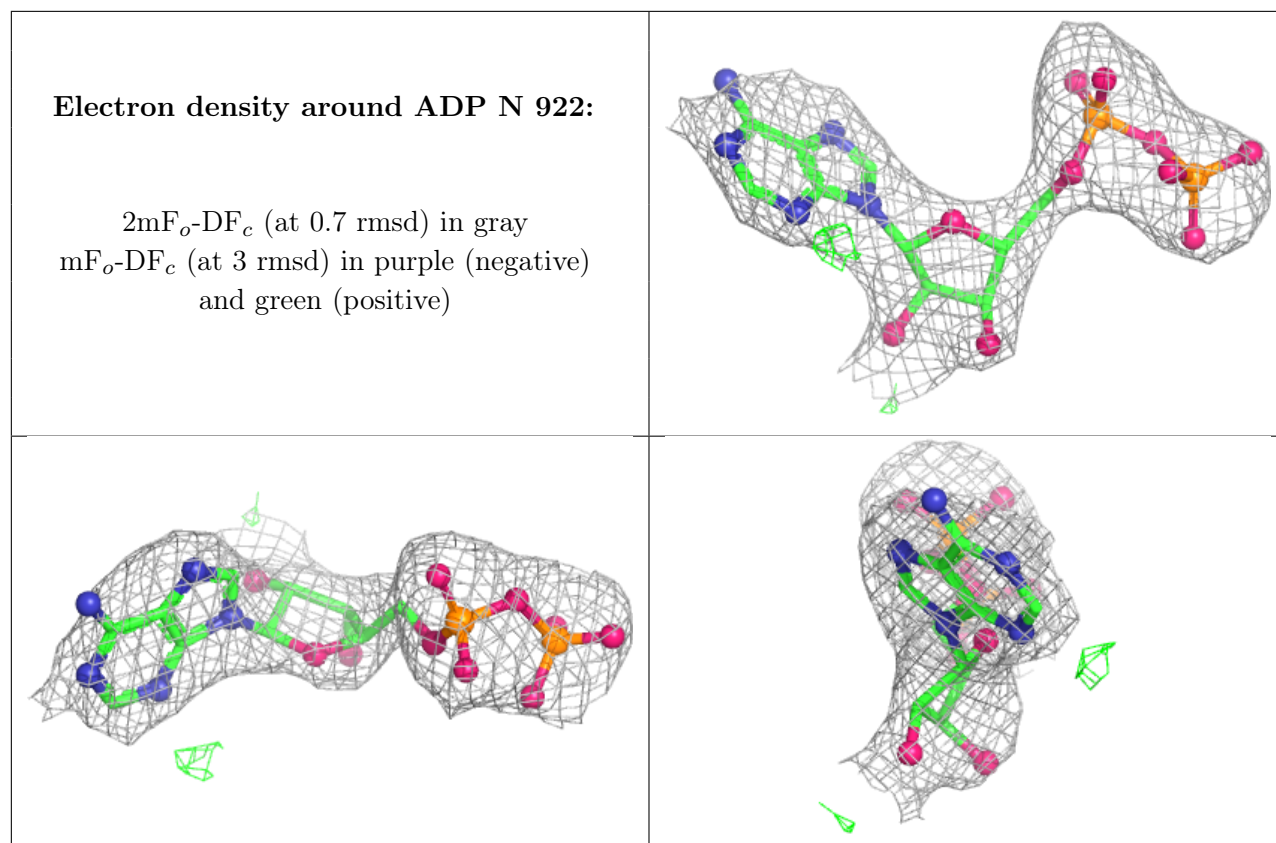
6.4 Ligands ⓘ

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	ADP	N	921	27/27	0.84	0.11	62,64,70,71	0
2	GLC	N	918	12/12	0.93	0.08	32,34,36,39	0
2	GLC	N	919	12/12	0.96	0.07	29,33,37,37	0
4	ADP	N	922	27/27	0.96	0.06	41,47,59,60	0
3	PO4	N	920	5/5	0.98	0.07	37,38,40,41	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.