



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:39 pm BST

PDB ID : 1KJQ  
Title : Crystal structure of glycinamide ribonucleotide transformylase in complex with Mg-ADP  
Authors : Thoden, J.B.; Firestine, S.M.; Benkovic, S.J.; Holden, H.M.  
Deposited on : 2001-12-05  
Resolution : 1.05 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](mailto: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.

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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 : 2.11  
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) : 2.11

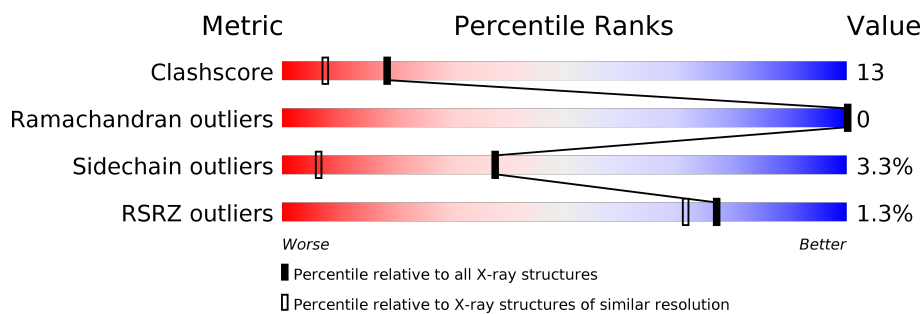
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.05 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	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	391	<div> <div>2%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
1	B	391	<div> <div>2%</div> <div>75%</div> <div>19%</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
7	EDO	A	400	-	-	X	-
7	EDO	A	407	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	EDO	B	398	-	-	X	-
7	EDO	B	399	-	-	X	-
7	EDO	B	401	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7204 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 phosphoribosylglycinamide formyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	15	0
			3019	1909	534	562	14			
1	B	385	Total	C	N	O	S	0	18	0
			3010	1905	530	561	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

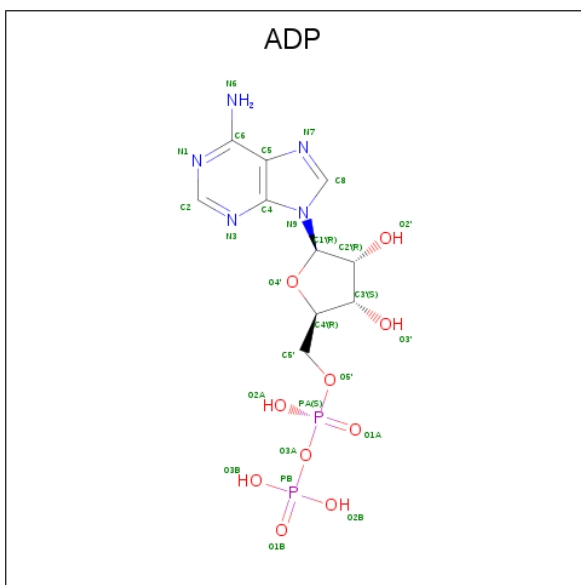
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

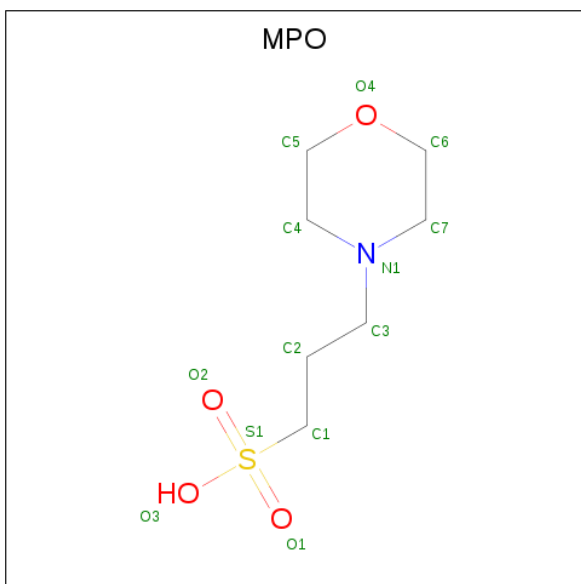
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula:  $C_7H_{15}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

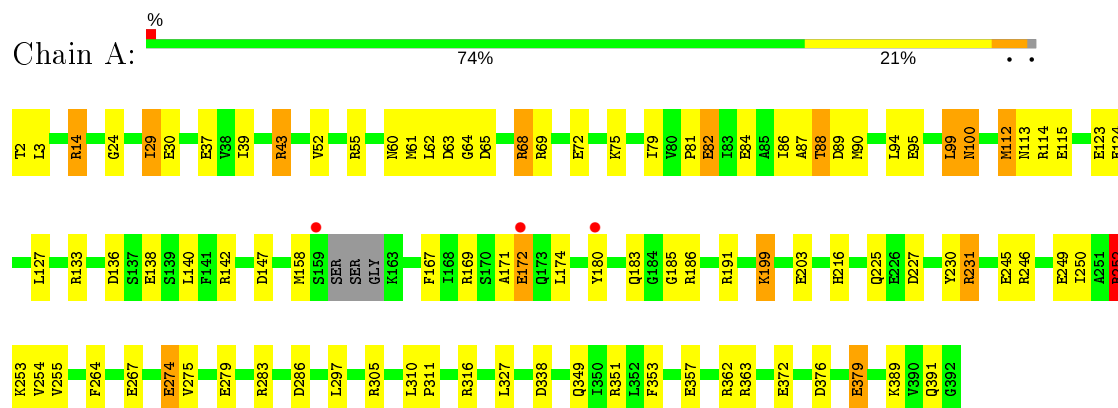
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	574	Total	O	0	10
			584	584		
8	B	444	Total	O	0	11
			456	456		

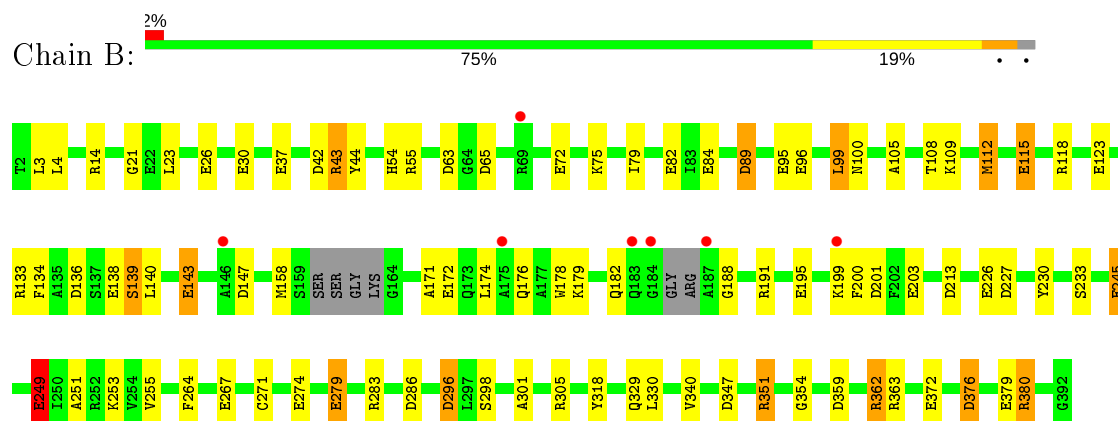
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: phosphoribosylglycinamide formyltransferase 2



- Molecule 1: phosphoribosylglycinamide formyltransferase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.35Å 179.34Å 75.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.05 28.46 – 1.05	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-1.05) 92.6 (28.46-1.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.65 (at 1.05Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.188 , 0.214 0.193 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 89.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7204	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ADP, CL, NA, EDO, MPO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.02	17/3128 (0.5%)	1.33	48/4237 (1.1%)
1	B	0.99	22/3138 (0.7%)	1.32	39/4253 (0.9%)
All	All	1.00	39/6266 (0.6%)	1.32	87/8490 (1.0%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	GLU	CD-OE2	7.94	1.34	1.25
1	B	245	GLU	CD-OE2	7.85	1.34	1.25
1	A	30	GLU	CD-OE2	7.12	1.33	1.25
1	B	138	GLU	CD-OE2	6.66	1.32	1.25
1	B	26	GLU	CD-OE2	6.61	1.32	1.25
1	A	95	GLU	CD-OE2	6.59	1.32	1.25
1	B	274	GLU	CD-OE2	6.46	1.32	1.25
1	B	95	GLU	CD-OE2	6.38	1.32	1.25
1	B	96	GLU	CD-OE2	6.32	1.32	1.25
1	A	115	GLU	CD-OE2	6.29	1.32	1.25
1	B	372	GLU	CD-OE2	6.27	1.32	1.25
1	A	372	GLU	CD-OE2	6.20	1.32	1.25
1	A	379	GLU	CD-OE2	6.19	1.32	1.25
1	A	172	GLU	CD-OE2	6.13	1.32	1.25
1	B	123	GLU	CD-OE2	6.13	1.32	1.25
1	A	123	GLU	CD-OE2	6.12	1.32	1.25
1	A	138	GLU	CD-OE2	6.08	1.32	1.25
1	B	203	GLU	CD-OE2	5.98	1.32	1.25
1	B	195	GLU	CD-OE2	5.86	1.32	1.25
1	B	84	GLU	CD-OE2	5.80	1.32	1.25
1	B	279[A]	GLU	CD-OE1	-5.64	1.19	1.25
1	B	279[B]	GLU	CD-OE1	-5.64	1.19	1.25
1	A	357	GLU	CD-OE1	-5.59	1.19	1.25
1	B	379	GLU	CD-OE2	5.57	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	GLU	CD-OE2	5.54	1.31	1.25
1	A	279	GLU	CD-OE2	5.54	1.31	1.25
1	B	267[A]	GLU	CD-OE2	5.50	1.31	1.25
1	B	267[B]	GLU	CD-OE2	5.50	1.31	1.25
1	B	72	GLU	CD-OE2	5.49	1.31	1.25
1	A	37	GLU	CD-OE2	5.47	1.31	1.25
1	A	274	GLU	CD-OE2	5.43	1.31	1.25
1	A	203	GLU	CD-OE2	5.34	1.31	1.25
1	A	245	GLU	CD-OE2	5.34	1.31	1.25
1	B	115	GLU	CD-OE2	5.33	1.31	1.25
1	B	172	GLU	CD-OE2	5.28	1.31	1.25
1	B	249	GLU	CD-OE2	5.24	1.31	1.25
1	B	226	GLU	CD-OE2	5.16	1.31	1.25
1	A	124	GLU	CD-OE2	5.14	1.31	1.25
1	B	143	GLU	CD-OE2	5.03	1.31	1.25

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363[A]	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	B	363[B]	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	B	43	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	180	TYR	CB-CG-CD2	-9.61	115.23	121.00
1	A	252[A]	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	252[B]	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	B	227	ASP	CB-CG-OD2	-9.04	110.16	118.30
1	A	363	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	B	43	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	316	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	B	305	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	316	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	68[A]	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	68[B]	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	133	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	118	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	B	136	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	B	286	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	A	376	ASP	CB-CG-OD2	-7.42	111.63	118.30
1	B	296	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	B	380[A]	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	B	380[B]	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	338	ASP	CB-CG-OD1	7.33	124.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	201	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	A	376	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	68[A]	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	68[B]	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	65	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	A	63	ASP	CB-CG-OD1	6.85	124.47	118.30
1	B	227	ASP	CB-CG-OD1	6.78	124.41	118.30
1	B	347	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	B	286	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	296	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	55	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	42	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	65	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	167	PHE	CB-CG-CD2	-6.32	116.38	120.80
1	A	286	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	180	TYR	CB-CG-CD1	6.29	124.77	121.00
1	B	363[A]	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	363[B]	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	283	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	136	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	231	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	147	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	227[A]	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	227[B]	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	191	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	167	PHE	CB-CG-CD1	6.00	125.00	120.80
1	B	65	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	63	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	89	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	363	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	286	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	351	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	136	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	351	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	376	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	213	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	252[A]	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	252[B]	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	362	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	359	ASP	CB-CG-OD1	5.53	123.27	118.30
1	B	44	TYR	CB-CG-CD1	-5.49	117.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	14	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	88	THR	N-CA-CB	-5.41	100.02	110.30
1	B	305	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	63	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	43	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	180	TYR	N-CA-CB	-5.31	101.05	110.60
1	A	136	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	233	SER	N-CA-CB	5.26	118.39	110.50
1	B	347	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	114	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	169	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	88	THR	CB-CA-C	5.18	125.60	111.60
1	A	338	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	118	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	231	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	283	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	353	PHE	N-CA-C	5.07	124.67	111.00
1	A	227[A]	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	227[B]	ASP	CB-CG-OD1	5.03	122.82	118.30
1	B	147	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	142	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	3019	0	3049	96	0
1	B	3010	0	3046	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	1	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	13	0	15	0	0
7	A	40	0	60	20	0
7	B	20	0	29	26	0
8	A	584	0	0	27	1
8	B	456	0	0	16	0
All	All	7204	0	6223	164	1

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 (164) 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:246:ARG:HD3	7:A:400:EDO:H21	1.27	1.09
1:A:94:LEU:HB3	1:A:99:LEU:HD22	1.27	1.07
1:B:301:ALA:HB2	7:B:398:EDO:H12	1.47	0.96
1:B:23:LEU:HB2	7:B:399:EDO:H12	1.53	0.90
1:B:140:LEU:HD22	7:B:401:EDO:H12	1.54	0.85
1:A:112[A]:MET:CE	1:A:113:ASN:HB2	2.08	0.84
1:A:99:LEU:HD12	8:A:960:HOH:O	1.78	0.83
1:A:275:VAL:H	7:A:400:EDO:H22	1.46	0.81
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.46	0.81
1:A:112[A]:MET:HE2	1:A:113:ASN:HB2	1.60	0.81
1:B:140:LEU:HB3	7:B:401:EDO:H11	1.64	0.79
1:B:105:ALA:O	1:B:108[A]:THR:HG22	1.83	0.78
1:A:310:LEU:HD21	1:B:340[A]:VAL:HG13	1.67	0.77
1:A:274:GLU:HA	7:A:400:EDO:H22	1.65	0.77
1:A:3:LEU:O	7:A:402:EDO:H22	1.85	0.76
1:B:178:TRP:O	1:B:182:GLN:HG2	1.85	0.75
1:A:14:ARG:HD3	8:A:553:HOH:O	1.88	0.73
1:A:43:ARG:NH2	8:A:809:HOH:O	2.11	0.73
1:A:2:THR:O	1:B:340[C]:VAL:HG22	1.87	0.73
1:A:87:ALA:HB1	7:A:407:EDO:O2	1.88	0.72
1:B:188:GLY:O	1:B:191:ARG:HG3	1.89	0.72
1:A:389[A]:LYS:HE3	1:A:391:GLN:CG	2.20	0.71
1:A:29[A]:ILE:HD11	1:A:52:VAL:HG11	1.73	0.71
1:A:389[A]:LYS:HE3	1:A:391:GLN:HG3	1.72	0.70
1:B:301:ALA:CB	7:B:398:EDO:H12	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:SER:O	1:B:143:GLU:HG3	1.93	0.69
1:B:140:LEU:CD2	7:B:401:EDO:H12	2.21	0.69
1:A:252[A]:ARG:HH22	1:A:253:LYS:HE3	1.58	0.68
1:A:39[A]:ILE:HD11	1:A:55:ARG:NH2	2.09	0.67
1:B:351:ARG:NH2	8:B:501:HOH:O	2.27	0.67
1:A:2:THR:HB	1:B:340[C]:VAL:HG23	1.76	0.66
1:B:23:LEU:CB	7:B:399:EDO:H12	2.23	0.66
1:B:251:ALA:O	1:B:255[B]:VAL:HG13	1.95	0.66
1:A:362:ARG:HG3	8:A:867[B]:HOH:O	1.97	0.65
1:B:298:SER:H	7:B:398:EDO:H11	1.62	0.65
1:A:69:ARG:HB3	7:A:401:EDO:H11	1.80	0.64
1:B:362:ARG:NH1	8:B:748:HOH:O	2.29	0.64
1:A:62:LEU:HD22	1:A:186:ARG:NH2	2.13	0.64
1:B:23:LEU:H	7:B:399:EDO:H11	1.61	0.64
1:B:380[A]:ARG:HG3	8:B:839:HOH:O	1.98	0.64
1:A:255[A]:VAL:HG23	1:A:264:PHE:CD1	2.33	0.63
1:B:279[B]:GLU:HG2	8:B:539:HOH:O	2.00	0.62
1:B:380[A]:ARG:HG2	8:B:740:HOH:O	1.99	0.62
1:A:29[A]:ILE:HD11	1:A:52:VAL:HG21	1.82	0.61
1:A:379:GLU:HG3	7:A:404:EDO:H12	1.81	0.61
8:A:452[B]:HOH:O	1:B:318:TYR:OH	2.15	0.60
1:A:79[B]:ILE:CD1	1:A:99:LEU:HD21	2.31	0.60
1:B:329:GLN:HG2	7:B:400:EDO:H12	1.81	0.60
1:A:29[A]:ILE:CD1	1:A:52:VAL:HG21	2.32	0.60
1:A:87:ALA:HB1	7:A:407:EDO:HO2	1.67	0.60
1:B:298:SER:H	7:B:398:EDO:C1	2.15	0.60
7:B:399:EDO:H21	8:B:807:HOH:O	2.02	0.59
1:A:90:MET:HB2	7:A:407:EDO:O2	2.03	0.59
1:B:23:LEU:H	7:B:399:EDO:C1	2.16	0.58
1:A:79[B]:ILE:HD11	1:A:99:LEU:HD21	1.85	0.58
7:B:402:EDO:H22	8:B:559:HOH:O	2.03	0.58
1:B:376:ASP:HB3	1:B:380[A]:ARG:HH11	1.67	0.58
1:A:2:THR:HB	1:B:340[A]:VAL:CG1	2.33	0.58
1:A:94:LEU:CB	1:A:99:LEU:HD22	2.19	0.58
1:A:186:ARG:NH1	8:A:899:HOH:O	2.36	0.57
1:A:112[A]:MET:HE3	1:A:158:MET:HG2	1.85	0.57
1:A:216:HIS:HD2	8:A:626:HOH:O	1.89	0.56
1:A:275:VAL:N	7:A:400:EDO:H22	2.17	0.55
1:A:112[A]:MET:HE1	1:A:158:MET:SD	2.46	0.55
1:B:100:ASN:ND2	8:B:647:HOH:O	2.39	0.55
1:B:298:SER:HB3	7:B:398:EDO:H11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLN:NE2	7:A:406:EDO:O2	2.35	0.55
1:A:61:MET:HG3	8:A:943:HOH:O	2.08	0.54
1:A:2:THR:O	1:B:340[A]:VAL:HG12	2.06	0.54
1:A:274:GLU:HG2	7:A:400:EDO:H12	1.89	0.54
1:A:379:GLU:HG3	7:A:404:EDO:C1	2.37	0.54
1:B:115:GLU:HG3	1:B:134:PHE:CZ	2.43	0.54
1:A:29[A]:ILE:HD11	1:A:52:VAL:CG1	2.38	0.53
1:A:185:GLY:HA3	8:A:953:HOH:O	2.08	0.53
1:A:29[A]:ILE:HD11	1:A:52:VAL:CB	2.38	0.53
1:B:329:GLN:HG2	7:B:400:EDO:C1	2.38	0.53
1:A:275:VAL:H	7:A:400:EDO:C2	2.17	0.52
1:B:179:LYS:O	1:B:182:GLN:HB2	2.09	0.52
1:A:250:ILE:O	1:A:254[A]:VAL:HG23	2.10	0.52
7:B:399:EDO:O1	8:B:714:HOH:O	2.19	0.52
1:B:354:GLY:N	4:B:396:CL:CL	2.78	0.52
1:B:21:GLY:C	7:B:399:EDO:H11	2.30	0.52
1:A:127:LEU:CD1	1:A:254[A]:VAL:HG22	2.40	0.51
1:B:376:ASP:HB3	1:B:380[A]:ARG:NH1	2.25	0.51
1:B:298:SER:CB	7:B:398:EDO:H11	2.41	0.51
1:A:75:LYS:NZ	8:A:861[A]:HOH:O	2.34	0.51
1:B:158:MET:HE3	1:B:188:GLY:HA2	1.93	0.51
1:B:200:PHE:HA	1:B:271[B]:CYS:SG	2.50	0.51
1:A:199:LYS:HE2	8:A:607:HOH:O	2.11	0.51
1:A:64:GLY:HA3	7:A:407:EDO:H12	1.93	0.50
1:A:112[A]:MET:HE2	1:A:113:ASN:CB	2.36	0.50
1:A:199:LYS:NZ	8:A:940:HOH:O	2.45	0.50
1:B:89:ASP:OD1	1:B:109:LYS:NZ	2.29	0.50
1:A:255[A]:VAL:HG23	1:A:264:PHE:CE1	2.47	0.50
1:B:3[A]:LEU:HD23	1:B:4:LEU:N	2.26	0.50
1:A:100:ASN:C	1:A:100:ASN:HD22	2.15	0.50
1:A:255[A]:VAL:CG2	1:A:264:PHE:CD1	2.95	0.50
1:B:158:MET:CE	1:B:188:GLY:HA2	2.42	0.50
1:B:249:GLU:HG2	8:B:834:HOH:O	2.11	0.49
1:A:14:ARG:NH1	8:A:553:HOH:O	2.18	0.49
1:A:112[A]:MET:CE	1:A:158:MET:SD	3.01	0.49
8:A:452[B]:HOH:O	1:B:296:ASP:HA	2.11	0.49
1:A:68[B]:ARG:NE	8:A:686:HOH:O	2.28	0.48
1:B:112:MET:HG3	1:B:112:MET:O	2.13	0.48
1:A:62:LEU:CD2	1:A:186:ARG:NH2	2.77	0.47
1:A:24:GLY:HA3	1:A:82[A]:GLU:OE2	2.14	0.47
1:A:81:PRO:HB3	1:A:86:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASN:HB2	7:A:403:EDO:H11	1.96	0.47
1:A:2:THR:HB	1:B:340[C]:VAL:CG2	2.40	0.47
1:B:43:ARG:CG	1:B:43:ARG:NH1	2.78	0.47
1:A:255[A]:VAL:CG2	1:A:264:PHE:CE1	2.98	0.47
7:A:399:EDO:O2	8:A:934:HOH:O	2.21	0.46
1:B:108[C]:THR:HG23	8:B:659:HOH:O	2.14	0.46
1:B:79:ILE:HD11	1:B:99:LEU:HD22	1.97	0.46
1:A:79[A]:ILE:HG13	1:A:99:LEU:CD2	2.45	0.46
1:A:186:ARG:HD2	8:A:899:HOH:O	2.15	0.46
1:A:255[A]:VAL:HG23	1:A:264:PHE:CG	2.51	0.46
1:B:30:GLU:OE1	7:B:398:EDO:H22	2.16	0.46
1:B:253:LYS:HB3	1:B:253:LYS:HE3	1.84	0.46
1:A:362:ARG:HG3	1:A:362:ARG:HH11	1.81	0.46
1:A:84:GLU:HG2	8:A:819:HOH:O	2.15	0.46
1:A:253:LYS:HD3	8:A:904:HOH:O	2.16	0.46
1:A:29[A]:ILE:HD11	1:A:52:VAL:CG2	2.45	0.45
1:B:43:ARG:NH1	1:B:43:ARG:HG2	2.16	0.45
1:B:140:LEU:HD22	7:B:401:EDO:C1	2.36	0.45
1:B:37:GLU:HA	1:B:54:HIS:CE1	2.51	0.45
1:B:14:ARG:HD3	8:B:823:HOH:O	2.17	0.45
1:A:127:LEU:HD11	1:A:254[A]:VAL:HG22	1.99	0.44
1:A:2:THR:HB	1:B:340[A]:VAL:HG13	1.98	0.44
1:A:2:THR:HB	1:B:340[A]:VAL:HG12	1.99	0.44
1:A:310:LEU:HD21	1:B:340[C]:VAL:HG23	1.99	0.44
1:A:305:ARG:HD3	1:A:311:PRO:O	2.18	0.44
1:B:176:GLN:HG3	8:B:641:HOH:O	2.17	0.43
1:A:225:GLN:NE2	8:A:528:HOH:O	2.41	0.43
1:A:79[B]:ILE:CD1	1:A:99:LEU:CD2	2.97	0.43
1:A:231:ARG:HH11	7:A:405:EDO:C1	2.31	0.43
1:A:112[A]:MET:HE2	1:A:113:ASN:N	2.33	0.43
7:B:402:EDO:H11	8:B:583:HOH:O	2.17	0.43
1:A:183:GLN:HB2	1:A:183:GLN:HE21	1.55	0.43
7:A:404:EDO:H21	8:A:675:HOH:O	2.18	0.43
1:B:30:GLU:OE1	7:B:398:EDO:C2	2.66	0.43
1:A:199:LYS:NZ	8:A:939:HOH:O	2.28	0.42
1:A:171:ALA:HA	1:A:174:LEU:HG	2.02	0.42
1:A:140:LEU:HD12	8:A:826:HOH:O	2.19	0.42
1:A:81:PRO:HB3	1:A:86:ILE:CD1	2.50	0.42
1:B:171:ALA:HA	1:B:174:LEU:HG	2.02	0.42
1:A:297:LEU:HD11	8:B:705:HOH:O	2.19	0.42
1:B:330:LEU:HA	7:B:400:EDO:O1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:N	7:B:399:EDO:H11	2.32	0.42
1:B:140:LEU:CB	7:B:401:EDO:H11	2.43	0.42
1:A:171:ALA:O	1:A:172:GLU:C	2.58	0.41
1:B:245:GLU:HG3	8:B:583:HOH:O	2.19	0.41
1:A:327:LEU:O	8:A:915:HOH:O	2.22	0.41
1:A:43:ARG:HB2	8:A:943:HOH:O	2.20	0.41
1:B:115:GLU:HG3	1:B:134:PHE:CE1	2.55	0.41
1:B:112:MET:CE	1:B:158:MET:SD	3.09	0.41
1:A:72[B]:GLU:HG2	8:A:815:HOH:O	2.20	0.41
1:A:231:ARG:HD2	7:A:405:EDO:H11	2.03	0.40
1:A:72[A]:GLU:HG2	8:A:815:HOH:O	2.20	0.40
1:B:255[A]:VAL:HG22	1:B:264:PHE:CG	2.55	0.40
1:A:62:LEU:HD22	1:A:186:ARG:HH21	1.84	0.40

All (1) 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)
4:A:395:CL:CL	8:A:699:HOH:O[4_455]	1.72	0.48

## 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	399/391 (102%)	388 (97%)	11 (3%)	0	100	100
1	B	399/391 (102%)	390 (98%)	9 (2%)	0	100	100
All	All	798/782 (102%)	778 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	323/311 (104%)	308 (95%)	15 (5%)	27	3
1	B	327/311 (105%)	318 (97%)	9 (3%)	43	9
All	All	650/622 (104%)	626 (96%)	24 (4%)	38	4

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29[A]	ILE
1	A	29[B]	ILE
1	A	82[A]	GLU
1	A	82[B]	GLU
1	A	88	THR
1	A	89	ASP
1	A	99	LEU
1	A	100	ASN
1	A	112[A]	MET
1	A	112[B]	MET
1	A	147	ASP
1	A	199	LYS
1	A	230	TYR
1	A	252[A]	ARG
1	A	252[B]	ARG
1	B	75	LYS
1	B	82	GLU
1	B	99	LEU
1	B	112	MET
1	B	133	ARG
1	B	139	SER
1	B	199	LYS
1	B	230	TYR
1	B	249	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	183	GLN
1	A	216	HIS
1	A	225	GLN
1	A	248	GLN
1	B	100	ASN
1	B	126	GLN
1	B	225	GLN
1	B	248	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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	$\# Z  > 2$
7	EDO	B	398	-	3,3,3	0.58	0	2,2,2	0.56	0
6	MPO	A	397	-	13,13,13	1.69	2 (15%)	17,17,17	1.37	2 (11%)
7	EDO	A	401	-	3,3,3	0.35	0	2,2,2	0.30	0
7	EDO	B	399	-	3,3,3	0.87	0	2,2,2	0.52	0
7	EDO	A	399	-	3,3,3	0.31	0	2,2,2	0.65	0
7	EDO	A	404	-	3,3,3	0.81	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	B	400	-	3,3,3	0.40	0	2,2,2	0.26	0
5	ADP	B	397	2	24,29,29	0.86	1 (4%)	29,45,45	1.71	6 (20%)
7	EDO	A	400	-	3,3,3	0.40	0	2,2,2	0.22	0
7	EDO	A	407	-	3,3,3	0.37	0	2,2,2	0.50	0
7	EDO	A	398	-	3,3,3	0.78	0	2,2,2	0.35	0
7	EDO	A	406	-	3,3,3	0.51	0	2,2,2	0.85	0
7	EDO	A	403	-	3,3,3	0.47	0	2,2,2	0.31	0
7	EDO	A	402	-	3,3,3	0.62	0	2,2,2	0.31	0
7	EDO	B	402	-	3,3,3	0.49	0	2,2,2	0.57	0
5	ADP	A	1	2	24,29,29	0.82	1 (4%)	29,45,45	1.51	4 (13%)
7	EDO	B	401	-	3,3,3	0.34	0	2,2,2	0.40	0
7	EDO	A	405	-	3,3,3	0.57	0	2,2,2	0.20	0

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
7	EDO	B	398	-	-	0/1/1/1	-
6	MPO	A	397	-	-	0/7/15/15	0/1/1/1
7	EDO	A	401	-	-	0/1/1/1	-
7	EDO	B	399	-	-	0/1/1/1	-
7	EDO	A	399	-	-	1/1/1/1	-
7	EDO	A	404	-	-	0/1/1/1	-
7	EDO	B	400	-	-	1/1/1/1	-
5	ADP	B	397	2	-	1/12/32/32	0/3/3/3
7	EDO	A	400	-	-	1/1/1/1	-
7	EDO	A	407	-	-	0/1/1/1	-
7	EDO	A	398	-	-	0/1/1/1	-
7	EDO	A	406	-	-	0/1/1/1	-
7	EDO	A	403	-	-	0/1/1/1	-
7	EDO	A	402	-	-	1/1/1/1	-
7	EDO	B	402	-	-	1/1/1/1	-
5	ADP	A	1	2	-	4/12/32/32	0/3/3/3
7	EDO	B	401	-	-	1/1/1/1	-
7	EDO	A	405	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	397	MPO	C3-N1	4.57	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	397	MPO	C1-S1	2.65	1.81	1.77
5	A	1	ADP	C2-N1	2.27	1.38	1.33
5	B	397	ADP	PB-O3B	2.06	1.62	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	397	ADP	C2-N1-C6	4.31	126.13	118.75
5	B	397	ADP	C5-C6-N1	-4.22	110.80	120.35
5	A	1	ADP	C5-C6-N6	3.99	126.41	120.35
5	B	397	ADP	N3-C2-N1	-3.40	123.36	128.68
5	A	1	ADP	C5-C6-N1	-3.11	113.29	120.35
5	B	397	ADP	N6-C6-N1	2.93	124.65	118.57
5	A	1	ADP	N3-C2-N1	-2.82	124.27	128.68
5	B	397	ADP	C5-C6-N6	2.76	124.55	120.35
5	A	1	ADP	C2-N1-C6	2.66	123.31	118.75
6	A	397	MPO	O3-S1-C1	2.63	110.03	105.77
6	A	397	MPO	C2-C3-N1	-2.58	107.33	113.84
5	B	397	ADP	C4-C5-N7	2.11	111.59	109.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	ADP	PA-O3A-PB-O3B
7	B	402	EDO	O1-C1-C2-O2
7	B	401	EDO	O1-C1-C2-O2
7	A	399	EDO	O1-C1-C2-O2
5	A	1	ADP	PA-O3A-PB-O2B
7	A	400	EDO	O1-C1-C2-O2
7	B	400	EDO	O1-C1-C2-O2
5	A	1	ADP	PB-O3A-PA-O1A
5	A	1	ADP	PA-O3A-PB-O1B
7	A	402	EDO	O1-C1-C2-O2
5	B	397	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

14 monomers are involved in 46 short contacts:

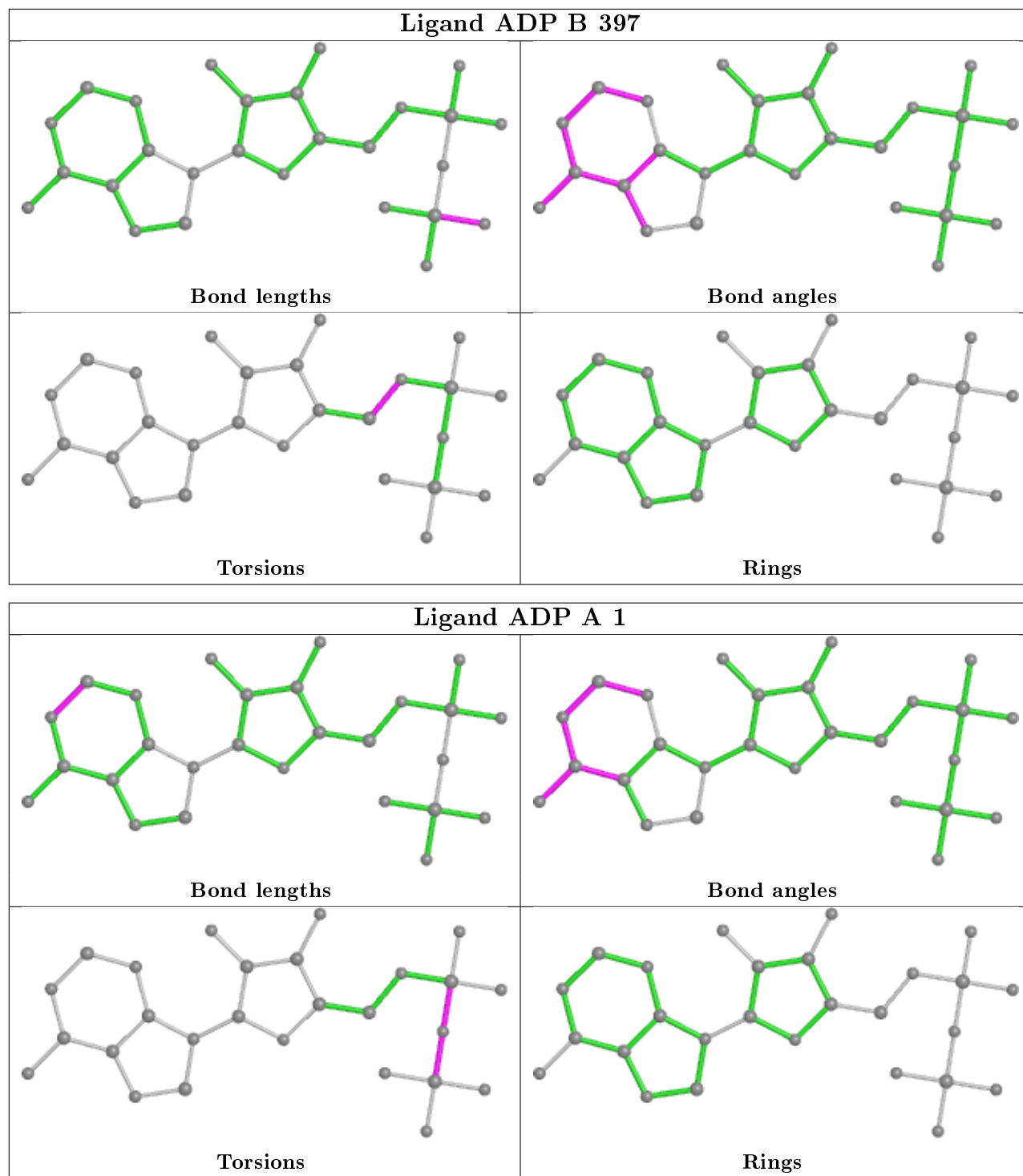
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	398	EDO	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	401	EDO	1	0
7	B	399	EDO	8	0
7	A	399	EDO	1	0
7	A	404	EDO	3	0
7	B	400	EDO	3	0
7	A	400	EDO	6	0
7	A	407	EDO	4	0
7	A	406	EDO	1	0
7	A	403	EDO	1	0
7	A	402	EDO	1	0
7	B	402	EDO	2	0
7	B	401	EDO	5	0
7	A	405	EDO	2	0

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



## 5.7 Other polymers ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/391 (99%)	-0.26	3 (0%) 86 82	7, 11, 32, 61	0
1	B	385/391 (98%)	-0.09	7 (1%) 68 62	7, 14, 45, 76	0
All	All	773/782 (98%)	-0.18	10 (1%) 77 71	7, 12, 41, 76	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	GLN	4.4
1	A	172	GLU	2.4
1	A	159	SER	2.4
1	A	180	TYR	2.4
1	B	184	GLY	2.3
1	B	146	ALA	2.3
1	B	69	ARG	2.2
1	B	175	ALA	2.1
1	B	187	ALA	2.1
1	B	199	LYS	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

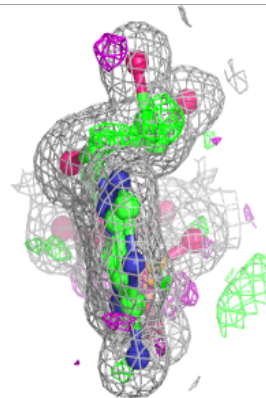
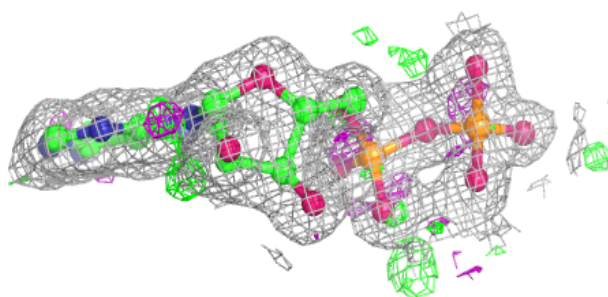
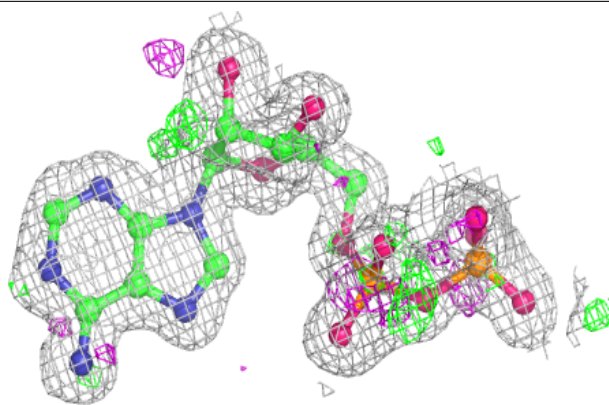
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	EDO	A	407	4/4	0.12	0.29	30,36,37,56	0
7	EDO	A	402	4/4	0.77	0.13	30,34,35,45	0
7	EDO	A	406	4/4	0.79	0.23	29,30,50,53	0
3	NA	B	394	1/1	0.80	0.21	20,20,20,20	0
7	EDO	B	401	4/4	0.82	0.10	35,36,37,41	0
7	EDO	A	404	4/4	0.83	0.19	18,33,41,46	0
7	EDO	B	400	4/4	0.84	0.20	20,27,28,64	0
7	EDO	B	402	4/4	0.85	0.15	33,51,70,96	0
7	EDO	B	399	4/4	0.86	0.16	8,18,32,32	0
7	EDO	A	405	4/4	0.87	0.18	30,37,49,49	0
7	EDO	A	399	4/4	0.88	0.11	31,36,39,46	0
7	EDO	A	403	4/4	0.90	0.09	24,25,29,37	0
7	EDO	A	401	4/4	0.90	0.14	29,45,53,56	0
7	EDO	B	398	4/4	0.92	0.14	19,20,31,69	0
3	NA	A	394	1/1	0.93	0.25	14,14,14,14	0
7	EDO	A	398	4/4	0.94	0.09	12,14,23,24	0
7	EDO	A	400	4/4	0.94	0.10	18,28,45,51	0
5	ADP	B	397	27/27	0.94	0.07	13,21,32,34	0
4	CL	B	395	1/1	0.97	0.04	21,21,21,21	0
4	CL	A	396	1/1	0.98	0.04	17,17,17,17	0
5	ADP	A	1	27/27	0.98	0.05	8,11,15,21	0
2	MG	A	393	1/1	0.98	0.04	12,12,12,12	0
4	CL	A	395	1/1	0.99	0.06	19,19,19,19	0
2	MG	B	393	1/1	0.99	0.06	19,19,19,19	0
4	CL	B	396	1/1	0.99	0.05	23,23,23,23	0
6	MPO	A	397	13/13	0.99	0.04	11,13,15,16	0

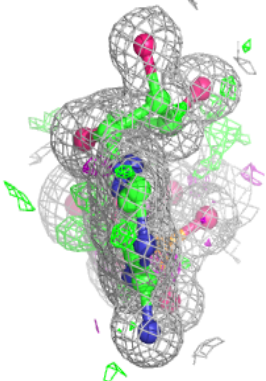
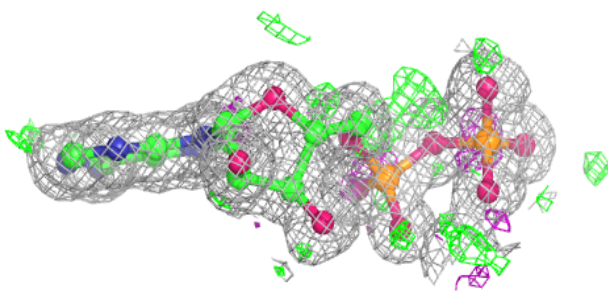
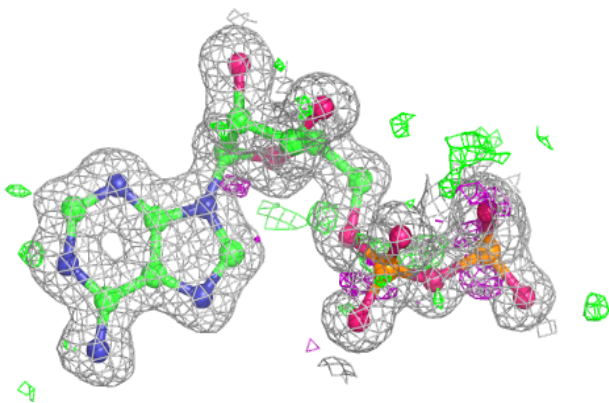
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP B 397:**

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

**Electron density around ADP A 1:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.