



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2017 – 11:25 PM EDT

PDB ID : 1KJJ  
Title : Crystal structure of glycylamide ribonucleotide transformylase in complex with Mg-ATP-gamma-S  
Authors : Thoden, J.B.; Firestone, S.M.; Benkovic, S.J.; Holden, H.M.  
Deposited on : unknown  
Resolution : 1.75 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

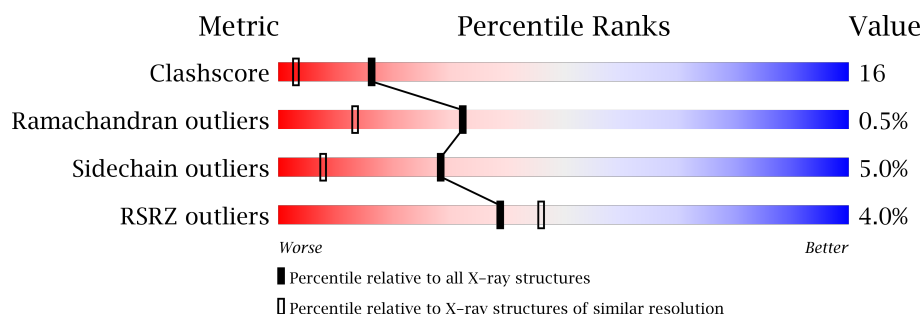
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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. 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	 70% 23% 5% ..
1	B	391	 60% 30% 8% ..

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6647 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	386	Total	C	N	O	S	0	1	0
			2949	1860	522	554	13			
1	B	385	Total	C	N	O	S	0	1	0
			2943	1855	521	553	14			

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

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

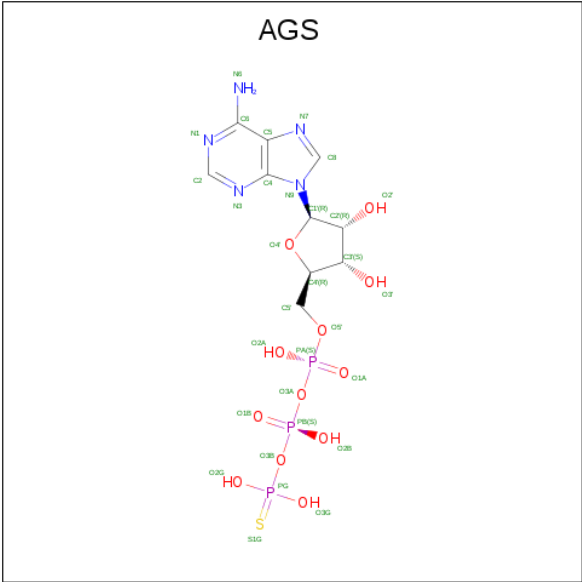
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

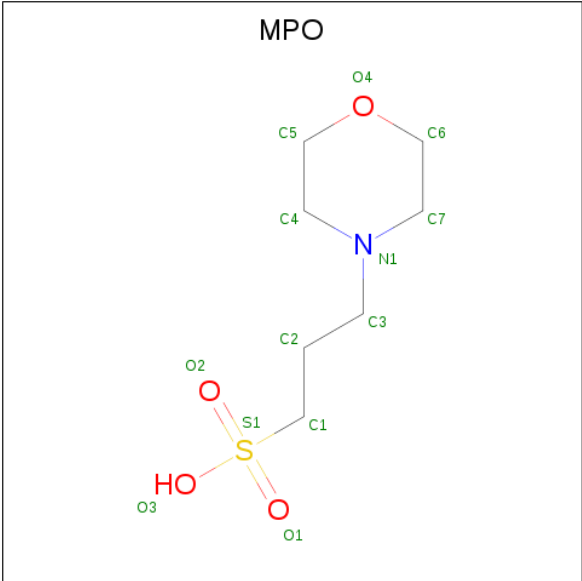
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



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

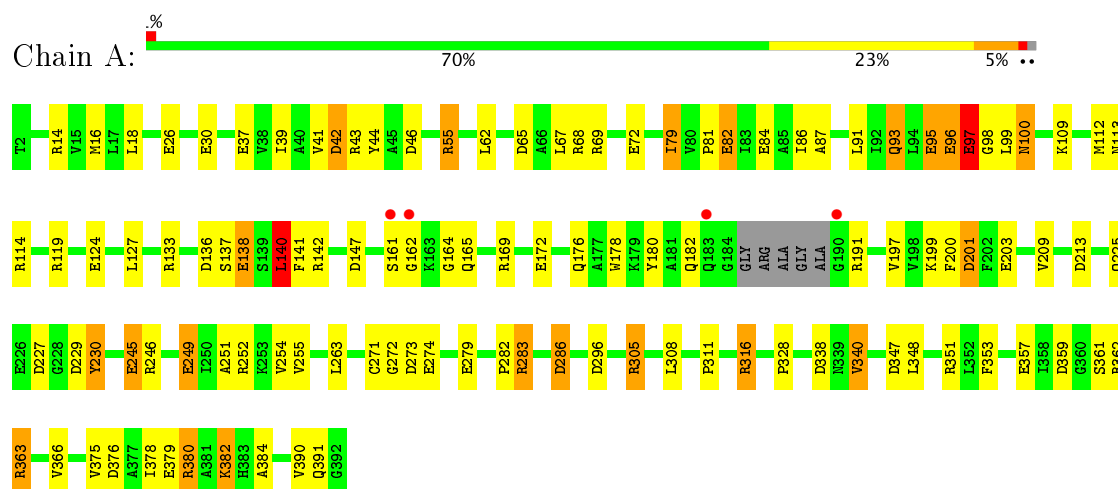
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	396	Total 396	O 396	0	0
7	B	278	Total 278	O 278	0	0

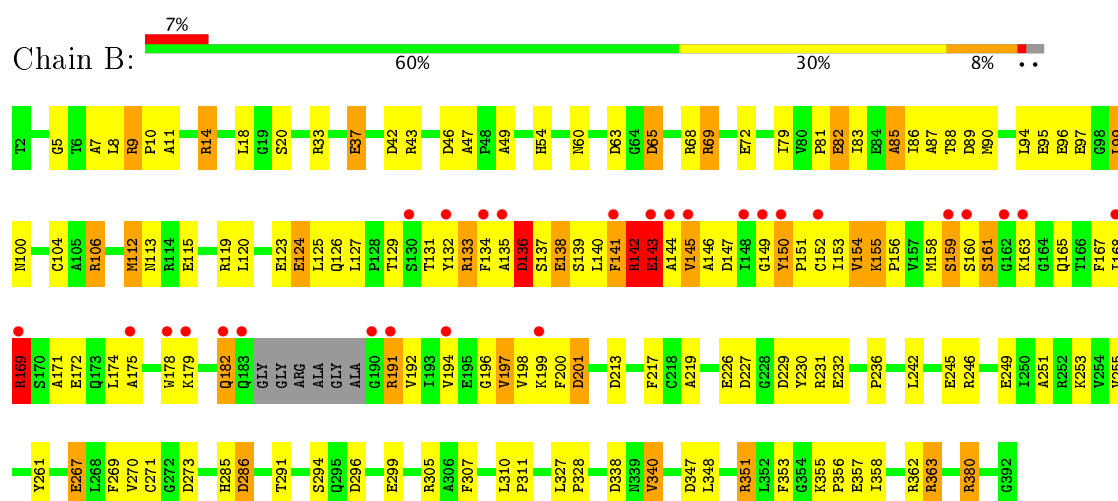
### 3 Residue-property plots [i](#)

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 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.90 Å   179.30 Å   76.10 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 1.75 50.94 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-1.75) 95.3 (50.94-1.75)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 1.75 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.184 ,      0.233 0.182 ,      (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 106.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: NA, MG, MPO, AGS, CL

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	19/3002 (0.6%)	1.57	57/4068 (1.4%)
1	B	0.99	17/2996 (0.6%)	1.55	48/4060 (1.2%)
All	All	1.00	36/5998 (0.6%)	1.56	105/8128 (1.3%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	GLU	CD-OE2	8.45	1.34	1.25
1	A	30	GLU	CD-OE2	8.39	1.34	1.25
1	B	172	GLU	CD-OE2	7.94	1.34	1.25
1	A	72	GLU	CD-OE2	7.56	1.33	1.25
1	B	226	GLU	CD-OE2	7.55	1.33	1.25
1	A	96	GLU	CD-OE2	7.23	1.33	1.25
1	B	143	GLU	CD-OE2	6.78	1.33	1.25
1	B	299	GLU	CD-OE1	-6.62	1.18	1.25
1	A	37	GLU	CD-OE2	6.61	1.32	1.25
1	B	97	GLU	CD-OE2	6.47	1.32	1.25
1	B	138	GLU	CD-OE2	6.33	1.32	1.25
1	B	82	GLU	CD-OE2	6.27	1.32	1.25
1	A	95	GLU	CD-OE2	6.08	1.32	1.25
1	A	84	GLU	CD-OE2	5.99	1.32	1.25
1	B	37	GLU	CD-OE1	-5.95	1.19	1.25
1	A	26	GLU	CD-OE2	5.94	1.32	1.25
1	B	267	GLU	CD-OE2	5.94	1.32	1.25
1	A	138	GLU	CD-OE2	5.84	1.32	1.25
1	A	279	GLU	CD-OE2	5.77	1.31	1.25
1	A	82	GLU	CD-OE2	5.75	1.31	1.25
1	B	249	GLU	CD-OE2	5.71	1.31	1.25
1	B	95	GLU	CD-OE2	5.69	1.31	1.25
1	A	245	GLU	CD-OE2	5.68	1.31	1.25
1	A	124	GLU	CD-OE2	5.65	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	GLU	CD-OE2	5.60	1.31	1.25
1	A	274	GLU	CD-OE2	5.58	1.31	1.25
1	B	357	GLU	CD-OE2	5.52	1.31	1.25
1	B	245	GLU	CD-OE2	5.45	1.31	1.25
1	A	249	GLU	CD-OE2	5.35	1.31	1.25
1	A	203	GLU	CD-OE2	5.32	1.31	1.25
1	B	72	GLU	CD-OE2	5.28	1.31	1.25
1	A	379	GLU	CD-OE2	5.26	1.31	1.25
1	A	172	GLU	CD-OE2	5.19	1.31	1.25
1	B	232	GLU	CD-OE1	-5.19	1.20	1.25
1	A	357	GLU	CD-OE2	5.07	1.31	1.25
1	B	124	GLU	CD-OE2	5.06	1.31	1.25

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ARG	NE-CZ-NH2	-12.71	113.95	120.30
1	A	363	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	B	191	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	A	286	ASP	CB-CG-OD1	10.52	127.77	118.30
1	A	136	ASP	CB-CG-OD2	-10.13	109.18	118.30
1	B	191	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	B	351	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	A	169	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	A	114	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	A	169	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	229	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	A	227	ASP	CB-CG-OD1	8.77	126.19	118.30
1	A	42	ASP	CB-CG-OD1	8.74	126.17	118.30
1	B	286	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	A	191	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	B	296	ASP	CB-CG-OD2	-8.45	110.70	118.30
1	B	296	ASP	CB-CG-OD1	8.31	125.78	118.30
1	B	363	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	A	119	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	347	ASP	CB-CG-OD1	8.11	125.60	118.30
1	B	286	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	283	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	340	VAL	CA-CB-CG1	-7.91	99.03	110.90
1	A	114	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	261	TYR	CB-CG-CD2	-7.81	116.31	121.00
1	B	133	ARG	NE-CZ-NH2	-7.76	116.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	ARG	CD-NE-CZ	7.63	134.28	123.60
1	A	42	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	316	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	B	14	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	286	ASP	CB-CG-OD2	-7.43	111.62	118.30
1	A	201	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	252	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	43	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	296	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	283	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	B	42	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	147	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	B	69	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	347	ASP	CB-CG-OD1	6.93	124.53	118.30
1	A	201	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	B	33	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	305	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	A	65	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	359	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	B	347	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	B	89	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	380	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	B	363	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	B	65	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	14	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	89	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	201	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	42	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	227	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	296	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	B	46	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	246	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	229	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	133	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	273	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	B	273	ASP	CB-CG-OD1	6.05	123.74	118.30
1	B	33	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	65	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	213	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	213	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	136	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	136	ASP	CB-CG-OD1	5.80	123.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	65	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	305	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	273	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	213	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	44	TYR	CB-CG-CD1	5.73	124.44	121.00
1	B	285	HIS	N-CA-CB	-5.73	100.29	110.60
1	A	197	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	A	69	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	230	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	B	227	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	B	217	PHE	CB-CA-C	-5.54	99.31	110.40
1	A	376	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	136	ASP	N-CA-CB	5.52	120.54	110.60
1	B	104	CYS	N-CA-CB	5.51	120.53	110.60
1	A	44	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	B	142	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	353	PHE	N-CA-C	5.50	125.84	111.00
1	A	213	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	9	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	227	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	140	LEU	CB-CG-CD1	-5.36	101.88	111.00
1	B	340	VAL	CA-CB-CG1	-5.29	102.97	110.90
1	B	380	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	140	LEU	N-CA-CB	-5.24	99.91	110.40
1	A	147	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	191	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	169	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	145	VAL	CA-CB-CG2	-5.20	103.09	110.90
1	A	376	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	338	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	55	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	79	ILE	CB-CA-C	5.04	121.69	111.60
1	B	43	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	46	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	231	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	353	PHE	N-CA-C	5.00	124.50	111.00

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	2949	0	2974	65	0
1	B	2943	0	2965	124	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	31	0	12	2	0
5	B	31	0	12	1	0
6	A	13	0	15	0	0
7	A	396	0	0	6	0
7	B	278	0	0	10	1
All	All	6647	0	5978	191	2

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 16.

All (191) 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:B:79:ILE:HD11	1:B:99:LEU:HD22	1.32	1.06
1:B:94:LEU:HB3	1:B:99:LEU:HD13	1.50	0.94
1:B:348:LEU:HB2	1:B:380:ARG:HH11	1.35	0.90
1:B:156:PRO:HG2	1:B:159:SER:HB2	1.52	0.90
1:B:161:SER:HB2	1:B:163:LYS:HE3	1.52	0.89
1:A:93:GLN:HA	1:A:93:GLN:HE21	1.40	0.85
1:B:191:ARG:HG3	1:B:192:VAL:N	1.99	0.78
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.47	0.77
1:B:153:ILE:CD1	1:B:197:VAL:HG22	2.14	0.76
1:A:99:LEU:HB2	7:A:625:HOH:O	1.86	0.76
1:B:141:PHE:CE1	1:B:145:VAL:HG21	2.20	0.76
1:B:156:PRO:HG2	1:B:159:SER:CB	2.16	0.75
1:A:18:LEU:HG	1:A:79:ILE:HD11	1.69	0.74
1:B:153:ILE:HD11	1:B:197:VAL:HG22	1.71	0.73
1:B:348:LEU:HB2	1:B:380:ARG:NH1	2.01	0.73
1:B:132:TYR:O	1:B:133:ARG:HD2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ILE:O	1:A:382:LYS:HG3	1.89	0.72
1:B:143:GLU:O	1:B:146:ALA:HB3	1.88	0.72
1:B:150:TYR:HB3	1:B:151:PRO:HA	1.71	0.70
1:B:68:ARG:HB2	1:B:90:MET:HE3	1.73	0.70
1:B:171:ALA:HA	1:B:174:LEU:HD13	1.74	0.70
1:B:79:ILE:CD1	1:B:99:LEU:HD22	2.15	0.70
1:A:79:ILE:HB	1:A:99:LEU:HD21	1.71	0.69
1:B:140:LEU:HA	1:B:143:GLU:HB2	1.75	0.69
1:B:174:LEU:HD12	1:B:174:LEU:H	1.58	0.68
1:B:200:PHE:HA	1:B:271[B]:CYS:SG	2.33	0.68
1:B:65:ASP:O	1:B:69:ARG:HG3	1.94	0.68
1:B:141:PHE:HE1	1:B:145:VAL:HG21	1.57	0.67
1:B:154:VAL:HG23	1:B:194:VAL:HG22	1.76	0.67
1:A:16:MET:O	1:A:79:ILE:HD12	1.93	0.67
1:B:161:SER:CB	1:B:163:LYS:HE3	2.26	0.66
1:B:79:ILE:HD11	1:B:99:LEU:CD2	2.17	0.66
1:B:174:LEU:N	1:B:174:LEU:HD12	2.10	0.66
1:B:88:THR:HG21	1:B:112:MET:HG2	1.78	0.66
1:A:16:MET:HB3	1:A:79:ILE:HD13	1.79	0.65
1:A:316:ARG:HD3	7:B:556:HOH:O	1.94	0.65
1:B:171:ALA:O	1:B:174:LEU:HD13	1.97	0.65
1:B:178:TRP:O	1:B:182:GLN:NE2	2.28	0.64
1:B:348:LEU:HD22	1:B:380:ARG:NH1	2.12	0.64
1:A:178:TRP:O	1:A:182:GLN:HG2	1.98	0.63
1:A:209:VAL:HG22	1:A:263:LEU:HD12	1.80	0.63
1:B:135:ALA:O	1:B:191:ARG:HD3	1.99	0.63
1:A:164:GLY:HA2	1:A:180:TYR:CE1	2.34	0.62
1:B:169:ARG:HG3	1:B:169:ARG:HH11	1.65	0.62
1:A:380:ARG:NH1	1:A:380:ARG:HG3	2.13	0.62
1:B:81:PRO:HB3	1:B:86:ILE:CD1	2.30	0.61
1:B:171:ALA:C	1:B:174:LEU:HD13	2.20	0.61
1:A:82:GLU:HB2	7:A:433:HOH:O	2.00	0.61
1:B:115:GLU:HG3	1:B:134:PHE:CE2	2.36	0.61
1:B:138:GLU:OE2	1:B:142:ARG:NH1	2.33	0.61
1:B:150:TYR:CE2	1:B:168:ILE:HG22	2.35	0.61
1:B:138:GLU:O	1:B:142:ARG:HB2	2.02	0.60
1:B:138:GLU:HA	1:B:141:PHE:HB3	1.84	0.60
1:A:200:PHE:HA	1:A:271:CYS:SG	2.42	0.59
1:B:115:GLU:HA	1:B:134:PHE:CZ	2.37	0.59
1:A:127:LEU:HD11	1:A:254:VAL:HG23	1.83	0.59
1:B:9:ARG:HB3	1:B:10:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASP:N	1:B:136:ASP:OD2	2.35	0.59
1:A:375:VAL:HG23	7:A:725:HOH:O	2.02	0.58
1:B:20:SER:HB3	1:B:49:ALA:HB3	1.85	0.58
1:B:153:ILE:HD12	1:B:197:VAL:HG22	1.85	0.57
1:A:39[A]:ILE:HD11	1:A:55:ARG:NH2	2.19	0.57
1:B:174:LEU:CD1	1:B:174:LEU:H	2.17	0.57
1:B:106:ARG:HD3	7:B:591:HOH:O	2.04	0.56
1:B:137:SER:O	1:B:141:PHE:N	2.29	0.56
1:B:127:LEU:HD21	1:B:253:LYS:HD2	1.87	0.56
1:B:9:ARG:HB3	1:B:10:PRO:CD	2.35	0.56
1:B:115:GLU:O	1:B:119:ARG:HG3	2.06	0.56
1:B:253:LYS:HG3	7:B:616:HOH:O	2.07	0.55
1:B:155:LYS:HG2	1:B:165:GLN:HG3	1.88	0.55
1:B:171:ALA:HA	1:B:174:LEU:CD1	2.37	0.55
1:B:174:LEU:O	1:B:175:ALA:C	2.44	0.55
1:A:251:ALA:O	1:A:255:VAL:HG13	2.06	0.54
1:B:115:GLU:HG3	1:B:134:PHE:CD2	2.41	0.54
1:B:150:TYR:CB	1:B:151:PRO:HA	2.33	0.54
1:B:242:LEU:HD21	1:B:246:ARG:NH1	2.23	0.53
1:A:100:ASN:HD22	1:A:100:ASN:C	2.12	0.53
1:A:137:SER:OG	1:A:140:LEU:HB2	2.09	0.53
1:B:348:LEU:HD22	1:B:380:ARG:HH11	1.73	0.52
1:A:93:GLN:HA	1:A:93:GLN:NE2	2.19	0.52
1:B:219:ALA:HB1	1:B:236:PRO:HB3	1.92	0.52
1:B:198:VAL:HA	7:B:609:HOH:O	2.11	0.51
1:B:199:LYS:HG3	1:B:199:LYS:O	2.10	0.51
1:A:138:GLU:O	1:A:142:ARG:HG3	2.11	0.50
1:B:131:THR:OG1	1:B:196:GLY:HA3	2.10	0.50
1:A:16:MET:HG2	1:A:79:ILE:CD1	2.42	0.50
1:A:249:GLU:HB3	7:A:668:HOH:O	2.10	0.50
1:B:68:ARG:CB	1:B:90:MET:HE3	2.41	0.50
1:A:348:LEU:HD11	1:A:384:ALA:HB2	1.93	0.50
1:B:132:TYR:CD2	1:B:132:TYR:N	2.80	0.50
1:A:245:GLU:O	1:A:249:GLU:HG3	2.13	0.49
1:A:176:GLN:NE2	1:A:176:GLN:HA	2.27	0.49
1:A:286:ASP:OD2	1:A:363:ARG:NH2	2.43	0.49
1:B:362:ARG:HD2	7:B:577:HOH:O	2.12	0.49
1:A:127:LEU:CD1	1:A:254:VAL:HG23	2.42	0.49
1:B:37:GLU:HA	1:B:54:HIS:CE1	2.47	0.49
1:B:267:GLU:HG2	7:B:562:HOH:O	2.13	0.49
1:B:68:ARG:HE	1:B:90:MET:HE3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:HA	1:A:99:LEU:O	2.13	0.49
1:B:356:PRO:HD2	7:B:628:HOH:O	2.12	0.49
1:B:83:ILE:HD12	1:B:85:ALA:HB3	1.94	0.49
1:A:305:ARG:HD3	1:A:311:PRO:O	2.13	0.48
1:B:141:PHE:CD2	1:B:178:TRP:HB2	2.48	0.48
1:B:20:SER:CB	1:B:49:ALA:HB3	2.43	0.48
1:A:348:LEU:HD11	1:A:384:ALA:CB	2.43	0.48
1:B:171:ALA:CA	1:B:174:LEU:HD13	2.42	0.48
1:B:327:LEU:HD12	1:B:362:ARG:C	2.34	0.48
1:B:348:LEU:CB	1:B:380:ARG:HH11	2.16	0.48
1:A:328:PRO:HD2	1:A:362:ARG:O	2.14	0.47
1:B:127:LEU:O	1:B:129:THR:HG23	2.13	0.47
1:B:141:PHE:CE1	1:B:145:VAL:CG2	2.94	0.47
1:B:286:ASP:OD2	1:B:363:ARG:NH2	2.45	0.47
1:B:348:LEU:CD2	1:B:380:ARG:NH1	2.76	0.47
1:B:348:LEU:CB	1:B:380:ARG:NH1	2.74	0.47
1:B:113:ASN:ND2	1:B:158:MET:CE	2.78	0.47
1:B:113:ASN:ND2	1:B:158:MET:HE3	2.29	0.47
1:B:14:ARG:HG2	1:B:37:GLU:HB3	1.97	0.47
1:B:153:ILE:HD12	1:B:197:VAL:CG2	2.45	0.47
1:B:113:ASN:HD22	1:B:158:MET:CE	2.28	0.47
1:B:18:LEU:HB2	1:B:81:PRO:HA	1.96	0.47
1:B:113:ASN:HD22	1:B:158:MET:HE2	1.79	0.47
1:B:86:ILE:HG22	1:B:87:ALA:N	2.30	0.47
1:B:242:LEU:CD2	1:B:246:ARG:NH1	2.79	0.46
1:A:99:LEU:HG	1:A:100:ASN:N	2.30	0.46
1:B:137:SER:OG	1:B:140:LEU:HD12	2.14	0.46
5:A:1:AGS:O5'	5:A:1:AGS:H8	2.14	0.46
1:A:282:PRO:O	1:A:283:ARG:HB3	2.15	0.46
1:B:120:LEU:HD12	1:B:124:GLU:HB3	1.98	0.46
1:B:291:THR:HA	1:B:294:SER:OG	2.16	0.46
1:A:225:GLN:NE2	7:A:737:HOH:O	2.44	0.46
1:B:362:ARG:NH1	7:B:628:HOH:O	2.48	0.46
1:B:305:ARG:HD3	1:B:310:LEU:HB2	1.98	0.45
1:B:5:GLY:HA3	1:B:11:ALA:O	2.16	0.45
1:B:142:ARG:HG3	1:B:174:LEU:HD23	1.97	0.45
1:B:355:LYS:HD3	1:B:362:ARG:HE	1.82	0.45
1:B:60:ASN:O	1:B:63:ASP:HB3	2.16	0.45
1:B:81:PRO:HB3	1:B:86:ILE:HD13	1.96	0.45
1:A:93:GLN:NE2	1:A:96:GLU:OE1	2.49	0.45
1:B:151:PRO:HB2	1:B:167:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:HB3	1:A:86:ILE:HD12	1.99	0.45
1:A:162:GLY:HA2	1:A:165:GLN:NE2	2.32	0.45
1:B:251:ALA:O	1:B:255:VAL:HG13	2.16	0.45
1:B:149:GLY:O	1:B:152:CYS:HB3	2.16	0.45
1:A:79:ILE:CB	1:A:99:LEU:HD21	2.42	0.44
1:A:42:ASP:OD2	1:A:43:ARG:N	2.44	0.44
1:A:96:GLU:C	1:A:98:GLY:H	2.21	0.44
1:B:150:TYR:CE2	1:B:168:ILE:CG2	3.01	0.44
1:B:174:LEU:CD1	1:B:174:LEU:N	2.78	0.44
1:A:43:ARG:HG3	1:A:43:ARG:O	2.18	0.44
1:B:340:VAL:O	1:B:340:VAL:HG12	2.16	0.44
1:A:340:VAL:O	1:A:340:VAL:HG12	2.17	0.44
1:A:164:GLY:CA	1:A:180:TYR:CE1	3.01	0.44
1:A:161:SER:N	5:A:1:AGS:S1G	2.89	0.43
1:A:16:MET:CB	1:A:79:ILE:HD13	2.47	0.43
1:B:155:LYS:HE2	1:B:165:GLN:OE1	2.18	0.43
1:B:305:ARG:HD3	1:B:310:LEU:CB	2.48	0.43
1:A:390:VAL:C	1:A:391:GLN:HG3	2.39	0.43
1:B:119:ARG:O	1:B:123:GLU:HB2	2.17	0.43
1:A:18:LEU:HD23	1:A:41:VAL:HB	2.01	0.43
1:A:79:ILE:HD12	1:A:79:ILE:HA	1.55	0.43
1:B:358:ILE:HD12	1:B:362:ARG:HB3	2.01	0.43
5:B:395:AGS:O5'	5:B:395:AGS:H8	2.18	0.43
1:A:141:PHE:CE2	1:A:178:TRP:HB2	2.54	0.42
1:A:138:GLU:O	1:A:141:PHE:HB3	2.18	0.42
1:A:391:GLN:NE2	7:A:431:HOH:O	2.51	0.42
1:B:20:SER:HB2	1:B:47:ALA:HB3	2.01	0.42
1:B:305:ARG:HD2	1:B:311:PRO:O	2.19	0.42
1:B:328:PRO:HD2	1:B:362:ARG:O	2.20	0.42
1:B:68:ARG:HE	1:B:90:MET:CE	2.33	0.42
1:B:82:GLU:HB2	7:B:453:HOH:O	2.19	0.42
1:B:140:LEU:O	1:B:144:ALA:N	2.41	0.42
1:B:150:TYR:CD2	1:B:168:ILE:HG22	2.55	0.42
1:A:62:LEU:HA	1:A:62:LEU:HD23	1.86	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.76	0.41
1:B:200:PHE:CB	1:B:269:PHE:HB3	2.51	0.41
1:A:79:ILE:CG2	1:A:99:LEU:CD2	2.98	0.41
1:B:150:TYR:HA	1:B:151:PRO:C	2.41	0.41
1:A:351:ARG:HB2	1:A:366:VAL:HG12	2.01	0.41
1:A:67:LEU:HD12	1:A:67:LEU:HA	1.81	0.41
1:B:351:ARG:NH2	7:B:665:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:HG2	1:A:79:ILE:HD11	2.01	0.41
1:B:201:ASP:N	1:B:270:VAL:O	2.49	0.41
1:A:68:ARG:HH12	1:A:97:GLU:CD	2.23	0.41
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.95	0.41
1:B:125:LEU:O	1:B:126:GLN:HB2	2.21	0.41
1:B:68:ARG:NE	1:B:90:MET:HE3	2.36	0.41
1:A:81:PRO:HB3	1:A:86:ILE:CD1	2.52	0.40
1:B:141:PHE:CD1	1:B:141:PHE:C	2.95	0.40
1:A:201:ASP:OD1	1:A:272:GLY:N	2.53	0.40
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.92	0.40
1:B:7:ALA:O	1:B:8:LEU:HB2	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH2	1:B:191:ARG:NH2[2_555]	1.72	0.48
7:B:639:HOH:O	7:B:639:HOH:O[2_655]	1.86	0.34

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/391 (98%)	372 (97%)	9 (2%)	2 (0%)	32	13
1	B	382/391 (98%)	365 (96%)	15 (4%)	2 (0%)	32	13
All	All	765/782 (98%)	737 (96%)	24 (3%)	4 (0%)	32	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ALA

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Mol	Chain	Res	Type
1	A	97	GLU
1	B	85	ALA
1	B	197	VAL

### 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	311/311 (100%)	301 (97%)	10 (3%)	44	19
1	B	311/311 (100%)	290 (93%)	21 (7%)	18	3
All	All	622/622 (100%)	591 (95%)	31 (5%)	28	8

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	100	ASN
1	A	109	LYS
1	A	112	MET
1	A	113	ASN
1	A	140	LEU
1	A	199	LYS
1	A	230	TYR
1	A	361	SER
1	A	382	LYS
1	B	99	LEU
1	B	100	ASN
1	B	106	ARG
1	B	112	MET
1	B	136	ASP
1	B	139	SER
1	B	141	PHE
1	B	142	ARG
1	B	143	GLU
1	B	150	TYR

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Mol	Chain	Res	Type
1	B	154	VAL
1	B	155	LYS
1	B	159	SER
1	B	160	SER
1	B	161	SER
1	B	169	ARG
1	B	179	LYS
1	B	182	GLN
1	B	229	ASP
1	B	230	TYR
1	B	307	PHE

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

Mol	Chain	Res	Type
1	A	93	GLN
1	A	100	ASN
1	A	176	GLN
1	A	225	GLN
1	A	248	GLN
1	A	391	GLN
1	B	100	ASN
1	B	126	GLN
1	B	176	GLN
1	B	225	GLN
1	B	238	GLN
1	B	333	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

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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
5	AGS	A	1	2	26,33,33	2.57	2 (7%)	22,52,52	2.74	7 (31%)
6	MPO	A	397	-	13,13,13	2.13	3 (23%)	16,17,17	2.63	5 (31%)
5	AGS	B	395	2	26,33,33	2.46	2 (7%)	22,52,52	2.10	5 (22%)

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
5	AGS	A	1	2	-	0/17/38/38	0/3/3/3
6	MPO	A	397	-	-	0/7/15/15	0/1/1/1
5	AGS	B	395	2	-	0/17/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	AGS	PG-S1G	-12.16	1.67	1.90
5	B	395	AGS	PG-S1G	-11.78	1.68	1.90
6	A	397	MPO	O1-S1	2.14	1.51	1.45
5	A	1	AGS	C2-N1	2.52	1.38	1.33
5	B	395	AGS	C2-N1	2.53	1.38	1.33
6	A	397	MPO	C3-N1	4.44	1.57	1.47
6	A	397	MPO	C1-S1	4.99	1.84	1.77

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	AGS	N3-C2-N1	-8.72	121.27	128.86
6	A	397	MPO	O3-S1-O1	-6.71	95.99	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	395	AGS	N3-C2-N1	-4.33	125.09	128.86
5	A	1	AGS	C5-C6-N1	-3.26	109.84	119.70
5	B	395	AGS	C5-C6-N1	-2.94	110.80	119.70
5	A	1	AGS	PB-O3B-PG	-2.06	125.70	132.35
5	A	1	AGS	O3'-C3'-C2'	2.13	118.64	111.83
6	A	397	MPO	C5-C4-N1	2.27	113.29	110.11
6	A	397	MPO	O1-S1-C1	2.71	109.12	106.79
5	A	1	AGS	C4'-O4'-C1'	2.77	112.72	109.77
5	B	395	AGS	C4'-O4'-C1'	3.59	113.59	109.77
5	B	395	AGS	C2-N1-C6	3.75	125.33	118.77
5	A	1	AGS	C5-C6-N6	4.35	129.34	120.47
6	A	397	MPO	O2-S1-C1	4.54	110.69	106.79
6	A	397	MPO	O3-S1-C1	4.82	111.99	106.06
5	B	395	AGS	C5-C6-N6	5.16	130.99	120.47
5	A	1	AGS	C2-N1-C6	5.84	128.98	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	AGS	2	0
5	B	395	AGS	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	386/391 (98%)	-0.55	4 (1%) 82 88	14, 21, 53, 93	0
1	B	385/391 (98%)	-0.09	27 (7%) 17 23	13, 27, 80, 95	0
All	All	771/782 (98%)	-0.32	31 (4%) 39 46	13, 23, 71, 95	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	5.3
1	B	141	PHE	5.1
1	B	134	PHE	4.9
1	A	161	SER	4.7
1	B	150	TYR	4.6
1	A	162	GLY	4.4
1	B	163	LYS	4.1
1	B	169	ARG	4.0
1	B	162	GLY	3.0
1	B	182	GLN	2.9
1	B	159	SER	2.9
1	B	183	GLN	2.8
1	B	145	VAL	2.7
1	B	160	SER	2.7
1	B	190	GLY	2.6
1	B	144	ALA	2.6
1	B	199	LYS	2.6
1	B	148	ILE	2.6
1	B	178	TRP	2.5
1	B	168	ILE	2.5
1	B	132	TYR	2.4
1	B	143	GLU	2.4
1	A	190	GLY	2.4
1	B	191	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	179	LYS	2.3
1	A	183	GLN	2.1
1	B	194	VAL	2.1
1	B	149	GLY	2.1
1	B	130	SER	2.1
1	B	135	ALA	2.1
1	B	152	CYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	A	395	1/1	0.91	0.09	1.01	35,35,35,35	0
6	MPO	A	397	13/13	0.98	0.06	0.36	18,23,26,33	0
5	AGS	A	1	31/31	0.97	0.08	-0.24	15,22,64,71	0
2	MG	A	393	1/1	0.90	0.12	-0.29	46,46,46,46	0
4	CL	A	396	1/1	0.98	0.06	-0.33	28,28,28,28	0
5	AGS	B	395	31/31	0.92	0.10	-0.64	27,37,60,69	0
2	MG	B	393	1/1	0.96	0.08	-1.08	40,40,40,40	0
2	MG	B	394	1/1	0.95	0.09	-	39,39,39,39	0
2	MG	A	394	1/1	0.98	0.08	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.