



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:07 am BST

PDB ID : 1EZ1
Title : STRUCTURE OF ESCHERICHIA COLI PURT-ENCODED GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE COMPLEXED WITH MG, AMPPNP, AND GAR
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Deposited on : 2000-05-09
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

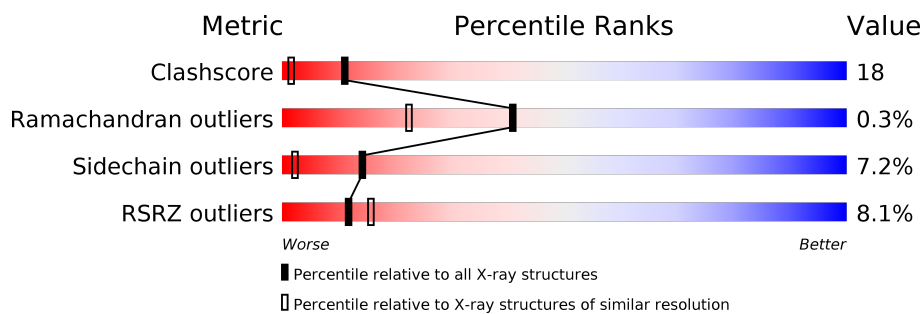
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.75 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	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	 <p>16% 71% 24% . .</p>
1	B	392	 <p>58% 32% 8% . .</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6992 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	389	Total	C	N	O	S	0	3	0
			2976	1873	529	561	13			
1	B	389	Total	C	N	O	S	0	1	0
			2972	1871	531	557	13			

- 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 ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

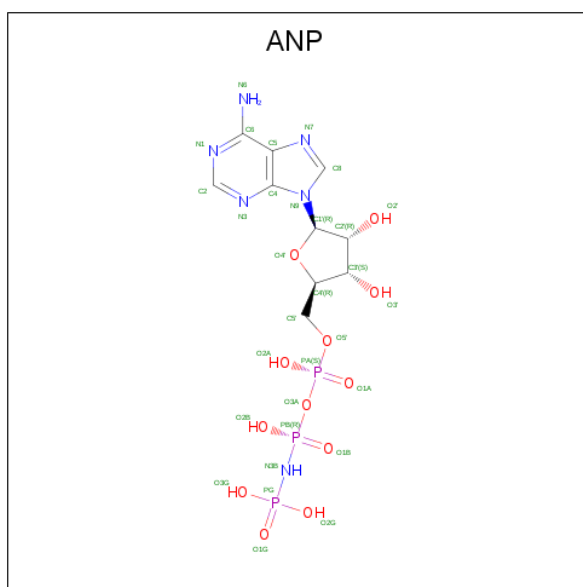


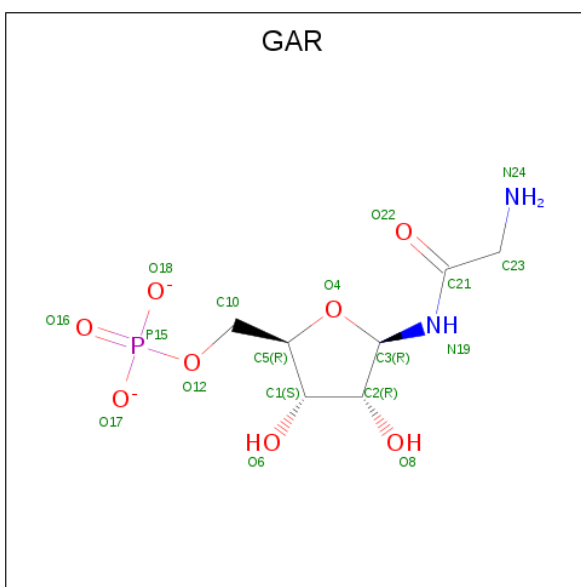
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

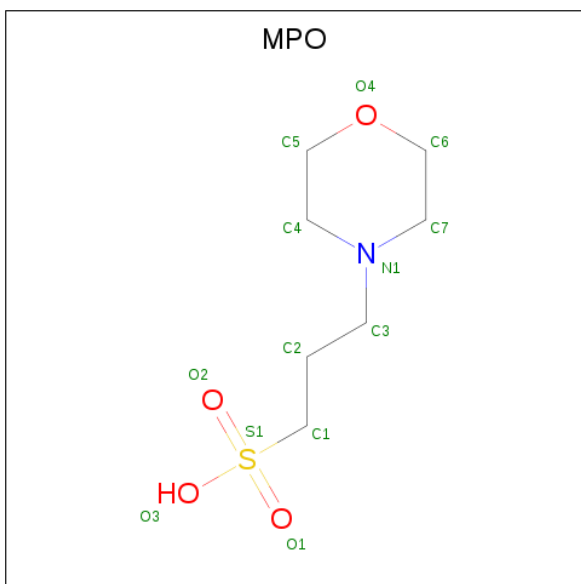
- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			18	7	2	8	1		
6	B	1	Total	C	N	O	P	0	0
			18	7	2	8	1		

- Molecule 7 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



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

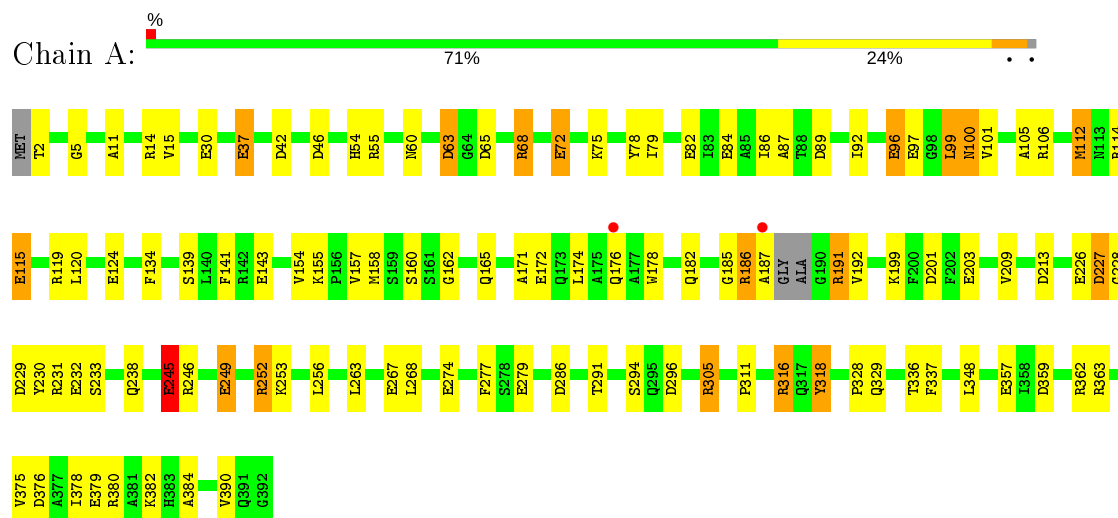
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	573	Total 573	O 573	0	0
8	B	346	Total 346	O 346	0	0

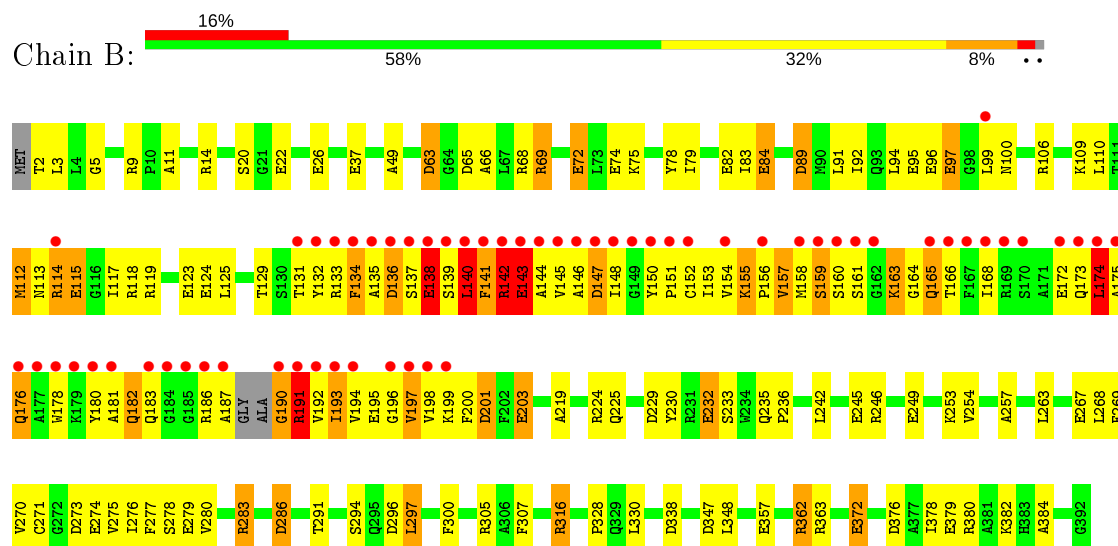
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	61.80 Å 179.40 Å 75.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 28.84 – 1.69	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-1.75) 93.8 (28.84-1.69)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 1.69 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.189 , 0.254 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 107.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6992	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NA, MPO, GAR, ANP, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.97	20/3037 (0.7%)	1.43	43/4114 (1.0%)
1	B	1.01	29/3025 (1.0%)	1.41	43/4097 (1.0%)
All	All	0.99	49/6062 (0.8%)	1.42	86/8211 (1.0%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	GLU	CD-OE2	8.10	1.34	1.25
1	B	143	GLU	CD-OE2	7.14	1.33	1.25
1	B	245	GLU	CD-OE2	7.10	1.33	1.25
1	B	203	GLU	CD-OE2	6.97	1.33	1.25
1	B	26	GLU	CD-OE2	6.95	1.33	1.25
1	A	96	GLU	CD-OE2	6.79	1.33	1.25
1	B	138	GLU	CD-OE2	6.73	1.33	1.25
1	B	172	GLU	CD-OE2	6.72	1.33	1.25
1	A	267	GLU	CD-OE2	6.26	1.32	1.25
1	A	232	GLU	CD-OE2	6.20	1.32	1.25
1	B	97	GLU	CD-OE2	6.11	1.32	1.25
1	B	249	GLU	CD-OE2	6.04	1.32	1.25
1	B	95	GLU	CD-OE2	6.01	1.32	1.25
1	B	141	PHE	CB-CG	5.97	1.61	1.51
1	A	30	GLU	CD-OE2	5.95	1.32	1.25
1	A	226	GLU	CD-OE2	5.94	1.32	1.25
1	B	115	GLU	CD-OE2	5.92	1.32	1.25
1	B	379	GLU	CD-OE2	5.85	1.32	1.25
1	A	115	GLU	CD-OE2	5.82	1.32	1.25
1	A	172	GLU	CD-OE2	5.82	1.32	1.25
1	B	372	GLU	CD-OE2	5.80	1.32	1.25
1	B	267	GLU	CD-OE2	5.78	1.32	1.25
1	B	357	GLU	CD-OE2	5.75	1.31	1.25
1	B	124	GLU	CD-OE2	5.72	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	GLU	CD-OE2	5.68	1.31	1.25
1	A	245	GLU	CD-OE2	5.66	1.31	1.25
1	A	379	GLU	CD-OE2	5.66	1.31	1.25
1	A	249	GLU	CD-OE2	5.65	1.31	1.25
1	B	82	GLU	CD-OE2	5.59	1.31	1.25
1	A	97	GLU	CD-OE2	5.57	1.31	1.25
1	B	22	GLU	CD-OE2	5.54	1.31	1.25
1	A	82	GLU	CD-OE2	5.54	1.31	1.25
1	B	279	GLU	CD-OE2	5.53	1.31	1.25
1	B	274	GLU	CD-OE2	5.52	1.31	1.25
1	B	232	GLU	CD-OE2	5.50	1.31	1.25
1	A	37	GLU	CD-OE2	5.49	1.31	1.25
1	B	96	GLU	CD-OE2	5.36	1.31	1.25
1	B	84	GLU	CD-OE2	5.32	1.31	1.25
1	A	203	GLU	CD-OE2	5.29	1.31	1.25
1	A	279	GLU	CD-OE2	5.28	1.31	1.25
1	B	72	GLU	CD-OE2	5.28	1.31	1.25
1	B	195	GLU	CD-OE2	5.23	1.31	1.25
1	A	357	GLU	CD-OE1	-5.21	1.20	1.25
1	B	37	GLU	CD-OE1	-5.09	1.20	1.25
1	A	279	GLU	CD-OE1	-5.07	1.20	1.25
1	B	37	GLU	CD-OE2	5.06	1.31	1.25
1	B	74	GLU	CD-OE2	5.04	1.31	1.25
1	A	357	GLU	CD-OE2	5.02	1.31	1.25
1	B	138	GLU	CD-OE1	-5.00	1.20	1.25

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH2	13.68	127.14	120.30
1	A	191	ARG	CD-NE-CZ	11.75	140.05	123.60
1	A	191	ARG	NE-CZ-NH1	-10.24	115.18	120.30
1	A	252	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	316	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	296	ASP	CB-CG-OD2	-8.84	110.35	118.30
1	A	296	ASP	CB-CG-OD1	8.47	125.93	118.30
1	B	305	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	B	197	VAL	C-N-CA	8.10	141.96	121.70
1	B	363	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	296	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	286	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	227[A]	ASP	CB-CG-OD1	7.86	125.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227[B]	ASP	CB-CG-OD1	7.86	125.38	118.30
1	B	197	VAL	CA-C-N	-7.71	100.23	117.20
1	B	296	ASP	CB-CG-OD1	7.55	125.10	118.30
1	B	191	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	114	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	213	ASP	CB-CG-OD1	7.36	124.92	118.30
1	B	65	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	376	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	B	286	ASP	CB-CG-OD1	7.02	124.62	118.30
1	B	376	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	213	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	B	201	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	A	55	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	89	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	227[A]	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	227[B]	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	201	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	283	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	A	201	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	B	197	VAL	O-C-N	6.53	133.15	122.70
1	A	55	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	305	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	305	ARG	CD-NE-CZ	-6.35	114.71	123.60
1	A	318	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	A	376	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	141	PHE	N-CA-CB	6.22	121.80	110.60
1	B	300	PHE	CB-CG-CD1	-6.21	116.45	120.80
1	A	316	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	134	PHE	CB-CG-CD2	6.12	125.08	120.80
1	A	362	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	65	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	286	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	273	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	89	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	B	140	LEU	N-CA-CB	6.00	122.40	110.40
1	A	286	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	63	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	316[A]	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	316[B]	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	42	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	233	SER	N-CA-CB	5.86	119.29	110.50
1	A	46	ASP	CB-CG-OD1	5.85	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	PHE	CB-CG-CD2	5.85	124.89	120.80
1	B	362	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	233	SER	N-CA-CB	5.83	119.24	110.50
1	A	46	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	347	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	380	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	14	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	140	LEU	C-N-CA	5.61	135.71	121.70
1	B	347	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	190	GLY	C-N-CA	5.59	135.68	121.70
1	A	359	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	359	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	245	GLU	CA-CB-CG	5.48	125.46	113.40
1	B	147	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	106	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	338	ASP	CB-CG-OD2	-5.31	113.53	118.30
1	B	9	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	224	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	246	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	65	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	363	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	106	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	142	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	63	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	186	ARG	CG-CD-NE	5.10	122.50	111.80
1	B	69	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	89	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	89	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	B	143	GLU	N-CA-CB	5.05	119.68	110.60
1	B	191	ARG	N-CA-CB	5.01	119.61	110.60
1	B	191	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	2976	0	2993	57	0
1	B	2972	0	2997	165	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	3	1	0
3	B	4	0	3	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	13	0	0
5	B	31	0	13	3	0
6	A	18	0	13	0	0
6	B	18	0	13	1	0
7	A	13	0	15	0	0
8	A	573	0	0	11	1
8	B	346	0	0	12	1
All	All	6992	0	6063	219	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 18.

All (219) 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:156:PRO:HG2	1:B:159:SER:HB2	1.42	1.01
1:B:148:ILE:HG13	1:B:194:VAL:HG12	1.43	0.99
1:B:136:ASP:HB3	1:B:191:ARG:NH1	1.80	0.94
1:A:158:MET:CE	1:A:186:ARG:HG3	1.98	0.93
1:B:174:LEU:H	1:B:174:LEU:HD23	1.34	0.91
1:B:197:VAL:HG22	5:B:1003:ANP:N1	1.86	0.90
1:B:141:PHE:CD2	1:B:178:TRP:HB2	2.05	0.90
1:B:141:PHE:HD2	1:B:178:TRP:HB2	1.39	0.86
1:A:158:MET:HE2	1:A:186:ARG:HG3	1.57	0.85
1:B:141:PHE:CE1	1:B:145:VAL:HG21	2.13	0.83
1:B:152:CYS:C	1:B:153:ILE:HD12	2.02	0.79
1:B:242:LEU:O	1:B:246:ARG:HG3	1.83	0.79
1:B:136:ASP:HB3	1:B:191:ARG:HH11	1.45	0.78
1:B:242:LEU:HD11	1:B:246:ARG:HE	1.48	0.78
1:B:297:LEU:HA	8:B:1527:HOH:O	1.84	0.77
1:B:156:PRO:CG	1:B:159:SER:HB2	2.17	0.75
1:B:153:ILE:HD13	1:B:197:VAL:HG23	1.67	0.75
1:B:174:LEU:N	1:B:174:LEU:HD23	2.01	0.75
1:B:269:PHE:CE2	1:B:278:SER:HB2	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:HG2	1:B:123:GLU:OE1	1.87	0.74
1:B:138:GLU:O	1:B:142:ARG:HB2	1.87	0.73
1:B:203:GLU:HG3	1:B:269:PHE:CD1	2.23	0.73
1:B:242:LEU:HD21	1:B:246:ARG:NH2	2.03	0.73
1:A:158:MET:HB3	1:A:186:ARG:NH1	2.02	0.73
1:B:232:GLU:CD	1:B:382:LYS:HD2	2.09	0.72
1:B:168:ILE:HG23	1:B:173:GLN:OE1	1.89	0.72
1:A:158:MET:HE3	1:A:186:ARG:HG3	1.71	0.71
1:B:113:ASN:ND2	1:B:115:GLU:HB3	2.06	0.70
1:B:242:LEU:HD11	1:B:246:ARG:NE	2.06	0.69
1:B:201:ASP:HB2	1:B:270:VAL:O	1.92	0.69
1:B:173:GLN:O	1:B:176:GLN:N	2.26	0.69
1:A:162:GLY:HA2	1:A:165:GLN:NE2	2.08	0.68
1:B:203:GLU:HG3	1:B:269:PHE:HD1	1.57	0.68
1:B:142:ARG:NH1	1:B:174:LEU:HB2	2.09	0.68
1:B:153:ILE:N	1:B:153:ILE:HD12	2.09	0.67
1:B:178:TRP:O	1:B:182:GLN:NE2	2.28	0.67
1:B:297:LEU:HD11	8:B:1796:HOH:O	1.93	0.67
1:A:155:LYS:HG2	1:A:165:GLN:HG3	1.76	0.67
1:A:165:GLN:NE2	8:A:1391:HOH:O	2.28	0.67
1:B:186:ARG:CG	1:B:187:ALA:H	2.06	0.67
1:B:193:ILE:HG13	1:B:194:VAL:N	2.08	0.66
1:B:316[B]:ARG:HD2	8:B:2206:HOH:O	1.96	0.65
1:B:69:ARG:NH2	8:B:1778:HOH:O	2.28	0.65
1:B:141:PHE:CE1	1:B:154:VAL:HG21	2.31	0.65
1:B:154:VAL:O	1:B:165:GLN:HA	1.97	0.65
1:B:14:ARG:HD3	8:B:2210:HOH:O	1.97	0.64
1:B:141:PHE:O	1:B:145:VAL:HG23	1.97	0.64
1:B:166:THR:HG22	1:B:168:ILE:HG13	1.80	0.64
1:B:150:TYR:CE2	1:B:168:ILE:HG22	2.33	0.64
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.61	0.64
1:B:160:SER:O	1:B:163:LYS:HB2	1.99	0.63
1:B:186:ARG:HG3	1:B:187:ALA:H	1.62	0.63
1:A:139:SER:O	1:A:143:GLU:HG3	1.99	0.63
1:B:141:PHE:HB2	1:B:178:TRP:CE3	2.33	0.62
1:B:142:ARG:CZ	1:B:174:LEU:HB2	2.30	0.62
1:A:100:ASN:C	1:A:100:ASN:HD22	2.02	0.61
1:B:173:GLN:O	1:B:176:GLN:HB2	2.00	0.61
1:B:182:GLN:N	1:B:182:GLN:HE21	1.99	0.60
1:A:75:LYS:NZ	8:A:1667:HOH:O	2.30	0.60
1:B:125:LEU:HD11	1:B:257:ALA:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:HA	1:B:117:ILE:HG22	1.85	0.59
1:B:145:VAL:HG13	1:B:152:CYS:SG	2.43	0.59
1:A:252:ARG:NH1	8:A:2203:HOH:O	2.36	0.58
1:B:113:ASN:HD21	1:B:115:GLU:HB3	1.67	0.58
1:A:171:ALA:HA	1:A:174:LEU:HG	1.85	0.58
1:B:150:TYR:HE2	1:B:168:ILE:HG22	1.69	0.57
1:B:132:TYR:N	1:B:132:TYR:CD2	2.72	0.57
1:B:277:PHE:CZ	1:B:280:VAL:HG12	2.40	0.57
1:B:277:PHE:HZ	1:B:280:VAL:HG12	1.69	0.57
1:A:100:ASN:HD22	1:A:101:VAL:N	2.03	0.56
1:B:14:ARG:NH1	8:B:2210:HOH:O	2.38	0.56
1:B:143:GLU:O	1:B:146:ALA:HB3	2.06	0.56
1:B:153:ILE:CG2	1:B:155:LYS:HE3	2.35	0.56
1:B:186:ARG:HG3	1:B:187:ALA:N	2.20	0.56
1:A:305:ARG:HD3	1:A:311:PRO:O	2.04	0.56
1:B:141:PHE:CD1	1:B:145:VAL:HG21	2.40	0.56
1:A:375:VAL:HG23	8:A:1725:HOH:O	2.06	0.56
1:A:348:LEU:HD11	1:A:384:ALA:CB	2.36	0.55
1:B:276:ILE:HD12	1:B:276:ILE:N	2.21	0.55
1:A:68:ARG:HG2	8:A:1664:HOH:O	2.06	0.55
1:B:137:SER:OG	1:B:140:LEU:HB2	2.08	0.54
1:B:153:ILE:CD1	1:B:197:VAL:HG23	2.38	0.54
1:B:63:ASP:HB3	1:B:66:ALA:HB3	1.90	0.54
1:A:79:ILE:HD11	1:A:99:LEU:HD22	1.90	0.54
1:B:137:SER:OG	1:B:140:LEU:N	2.37	0.54
1:B:283:ARG:NH2	8:B:1565:HOH:O	2.41	0.53
1:B:181:ALA:HB3	1:B:182:GLN:HE22	1.73	0.53
1:B:20:SER:HB3	1:B:49:ALA:HB3	1.91	0.53
1:B:380:ARG:NH1	1:B:380:ARG:HG3	2.23	0.53
1:B:145:VAL:HG22	1:B:194:VAL:HG21	1.90	0.53
1:B:137:SER:O	1:B:141:PHE:N	2.20	0.53
1:A:336:THR:HB	1:B:3:LEU:HD11	1.90	0.53
1:B:182:GLN:NE2	1:B:182:GLN:N	2.57	0.52
1:A:86:ILE:HG22	1:A:87:ALA:N	2.24	0.52
1:B:186:ARG:CG	1:B:187:ALA:N	2.72	0.52
1:B:268:LEU:HD23	1:B:277:PHE:HA	1.90	0.52
1:A:178:TRP:O	1:A:182:GLN:HG2	2.09	0.52
1:A:316:ARG:HD3	8:A:1556:HOH:O	2.09	0.52
1:B:254:VAL:HG11	1:B:280:VAL:HG11	1.92	0.52
1:B:84:GLU:OE2	1:B:112:MET:HA	2.10	0.51
1:B:242:LEU:HD11	1:B:246:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:TYR:CD2	1:B:100:ASN:ND2	2.79	0.51
1:B:173:GLN:O	1:B:175:ALA:N	2.44	0.51
1:A:92:ILE:O	1:A:96:GLU:HG3	2.11	0.51
1:A:162:GLY:HA2	1:A:165:GLN:HE22	1.76	0.50
1:A:185:GLY:C	1:A:187:ALA:H	2.13	0.50
1:B:131:THR:OG1	1:B:196:GLY:HA3	2.10	0.50
1:B:135:ALA:O	1:B:191:ARG:HD3	2.12	0.50
1:B:166:THR:HG22	1:B:168:ILE:CG1	2.41	0.50
1:B:142:ARG:HH12	1:B:174:LEU:C	2.15	0.50
1:A:99:LEU:HA	8:A:1493:HOH:O	2.11	0.50
1:B:232:GLU:CG	1:B:382:LYS:HD2	2.41	0.50
1:A:228:GLY:HA2	8:A:1696:HOH:O	2.12	0.49
1:B:144:ALA:O	1:B:147:ASP:HB2	2.12	0.49
1:B:191:ARG:HG3	1:B:192:VAL:N	2.24	0.49
1:B:144:ALA:O	1:B:147:ASP:N	2.46	0.49
1:B:115:GLU:HG3	1:B:134:PHE:CE1	2.47	0.49
1:B:328:PRO:HD2	1:B:362:ARG:O	2.12	0.49
1:B:148:ILE:CG1	1:B:194:VAL:HG12	2.28	0.49
1:B:242:LEU:HD11	1:B:246:ARG:HH21	1.76	0.49
1:A:231:ARG:HD2	8:A:1318:HOH:O	2.12	0.49
1:A:154:VAL:O	1:A:165:GLN:HA	2.13	0.49
1:A:141:PHE:CE2	1:A:178:TRP:HB2	2.47	0.48
1:A:191:ARG:HG2	1:A:192:VAL:N	2.28	0.48
1:A:348:LEU:HD11	1:A:384:ALA:HB2	1.93	0.48
1:B:154:VAL:HG23	1:B:194:VAL:HG22	1.94	0.48
1:B:99:LEU:HD13	8:B:2214:HOH:O	2.14	0.48
1:B:232:GLU:HG2	1:B:382:LYS:CD	2.44	0.48
1:B:150:TYR:HE2	1:B:168:ILE:CG2	2.27	0.48
1:B:197:VAL:HG13	1:B:198:VAL:N	2.28	0.48
1:B:348:LEU:HD11	1:B:384:ALA:CB	2.44	0.48
1:A:60:ASN:ND2	8:A:1652:HOH:O	2.47	0.48
1:A:328:PRO:HG3	1:A:390:VAL:HG11	1.96	0.47
1:B:153:ILE:CD1	1:B:197:VAL:CG2	2.92	0.47
1:A:120:LEU:HD12	1:A:124:GLU:HB2	1.96	0.47
1:B:232:GLU:HG2	1:B:382:LYS:HD2	1.96	0.47
1:A:84:GLU:HG2	1:A:112:MET:HA	1.96	0.47
1:B:166:THR:HG22	1:B:168:ILE:CD1	2.45	0.47
1:B:242:LEU:HD11	1:B:246:ARG:CZ	2.44	0.47
1:B:14:ARG:HH11	1:B:14:ARG:HG3	1.80	0.47
1:B:135:ALA:HB1	1:B:141:PHE:N	2.30	0.47
1:B:72:GLU:O	1:B:75:LYS:HE3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PRO:C	1:B:158:MET:H	2.18	0.47
1:A:268:LEU:HD23	1:A:277:PHE:HA	1.97	0.47
1:B:150:TYR:HA	1:B:151:PRO:HA	1.61	0.47
1:B:5:GLY:HA3	1:B:11:ALA:O	2.15	0.46
1:B:156:PRO:HD2	1:B:159:SER:CB	2.44	0.46
1:B:136:ASP:N	1:B:136:ASP:OD2	2.48	0.46
1:B:186:ARG:HD2	1:B:190:GLY:HA2	1.97	0.46
1:B:72:GLU:HA	1:B:75:LYS:HE3	1.97	0.46
1:A:185:GLY:C	1:A:187:ALA:N	2.69	0.46
1:A:245:GLU:O	1:A:249:GLU:HG3	2.16	0.45
1:B:180:TYR:HA	1:B:183:GLN:HB2	1.98	0.45
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.67	0.45
1:B:14:ARG:NH1	1:B:14:ARG:HG3	2.31	0.45
1:B:78:TYR:CE2	1:B:100:ASN:ND2	2.85	0.45
1:B:203:GLU:HG3	1:B:269:PHE:CE1	2.51	0.45
1:B:174:LEU:CD2	1:B:174:LEU:N	2.75	0.45
1:B:114:ARG:HE	1:B:114:ARG:HB3	1.65	0.45
1:B:148:ILE:HG13	1:B:194:VAL:CG1	2.29	0.45
1:B:91:LEU:HA	1:B:91:LEU:HD23	1.81	0.45
1:B:197:VAL:HG22	5:B:1003:ANP:C6	2.47	0.45
1:B:291:THR:HA	1:B:294:SER:OG	2.16	0.44
1:B:166:THR:CG2	1:B:168:ILE:HD11	2.47	0.44
1:A:176:GLN:NE2	8:A:2201:HOH:O	2.37	0.44
1:B:197:VAL:CG1	1:B:198:VAL:N	2.78	0.44
1:B:84:GLU:HG3	8:B:1780:HOH:O	2.18	0.44
1:B:153:ILE:HG22	1:B:155:LYS:HE3	1.98	0.44
1:B:242:LEU:HD21	1:B:246:ARG:CZ	2.48	0.44
1:B:203:GLU:CG	1:B:269:PHE:CD1	2.99	0.44
1:A:209:VAL:HG22	1:A:263:LEU:HD12	1.99	0.44
1:B:89:ASP:OD2	1:B:109:LYS:NZ	2.51	0.43
1:A:378:ILE:O	1:A:382:LYS:HG3	2.18	0.43
1:B:198:VAL:HG23	5:B:1003:ANP:HN62	1.83	0.43
1:B:200:PHE:HB3	1:B:269:PHE:HB3	1.99	0.43
1:B:2:THR:N	8:B:1202:HOH:O	2.50	0.43
1:A:318:TYR:O	1:B:316[B]:ARG:NH2	2.41	0.43
1:B:197:VAL:HA	1:B:198:VAL:HG23	2.01	0.43
1:A:92:ILE:HG13	1:A:105:ALA:HB1	2.01	0.43
1:B:129:THR:HA	1:B:276:ILE:CG2	2.49	0.43
1:B:235:GLN:HA	1:B:236:PRO:HA	1.82	0.43
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.85	0.43
1:A:134:PHE:HB3	1:A:191:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:N	3:A:960:ACT:OXT	2.52	0.42
1:B:156:PRO:HD3	1:B:164:GLY:O	2.19	0.42
1:B:131:THR:O	1:B:132:TYR:HB3	2.19	0.42
1:B:225:GLN:HB3	1:B:225:GLN:HE21	1.56	0.42
1:B:125:LEU:HD11	1:B:257:ALA:HB3	1.99	0.42
1:A:291:THR:HA	1:A:294:SER:OG	2.19	0.42
1:B:132:TYR:HA	1:B:194:VAL:O	2.20	0.42
1:A:15:VAL:HG22	1:A:78:TYR:HB2	2.01	0.42
1:B:135:ALA:HB1	1:B:140:LEU:C	2.39	0.42
1:B:153:ILE:N	1:B:153:ILE:CD1	2.81	0.42
1:B:219:ALA:HB1	1:B:236:PRO:HB3	2.02	0.42
1:B:79:ILE:HD11	1:B:99:LEU:HD12	2.02	0.42
1:A:5:GLY:HA3	1:A:11:ALA:O	2.19	0.42
1:B:378:ILE:HG22	1:B:382:LYS:HD3	2.01	0.42
1:A:157:VAL:HG23	1:A:158:MET:HG3	2.01	0.41
1:B:94:LEU:HA	1:B:94:LEU:HD23	1.85	0.41
1:B:142:ARG:NH1	1:B:174:LEU:CB	2.81	0.41
1:A:37:GLU:HA	1:A:54:HIS:CE1	2.55	0.41
1:B:316[B]:ARG:HD3	1:B:316[B]:ARG:HH11	1.64	0.41
1:B:68:ARG:HH12	1:B:97:GLU:CD	2.24	0.41
1:B:157:VAL:C	1:B:158:MET:HG2	2.41	0.41
1:B:166:THR:O	1:B:168:ILE:HD12	2.19	0.41
1:A:68:ARG:HD3	1:A:72:GLU:OE1	2.20	0.41
1:B:132:TYR:CE1	1:B:134:PHE:CE2	3.09	0.41
1:B:286:ASP:OD2	6:B:411:GAR:N24	2.53	0.41
1:B:114:ARG:HB3	8:B:2225:HOH:O	2.19	0.41
1:B:135:ALA:CB	1:B:141:PHE:HA	2.51	0.41
1:B:275:VAL:C	1:B:276:ILE:HD12	2.41	0.41
1:B:181:ALA:HB3	1:B:182:GLN:NE2	2.36	0.41
1:A:60:ASN:OD1	1:A:63:ASP:N	2.54	0.40
1:A:68:ARG:O	1:A:72:GLU:HG3	2.20	0.40
1:B:153:ILE:HD13	1:B:197:VAL:CG2	2.42	0.40
1:A:337:PHE:O	1:B:3:LEU:HD12	2.21	0.40
1:B:118:ARG:NE	8:B:1510:HOH:O	2.40	0.40
1:A:115:GLU:O	1:A:119:ARG:HG3	2.21	0.40
1:B:191:ARG:HD2	1:B:192:VAL:O	2.21	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)
8:B:1459:HOH:O	8:B:1459:HOH:O[2_655]	2.14	0.06
8:A:1101:HOH:O	8:A:1651:HOH:O[4_556]	2.17	0.03

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	388/392 (99%)	380 (98%)	8 (2%)	0	100	100
1	B	386/392 (98%)	364 (94%)	20 (5%)	2 (0%)	29	12
All	All	774/784 (99%)	744 (96%)	28 (4%)	2 (0%)	41	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	LEU
1	B	176	GLN

5.3.2 Protein sidechains [i](#)

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	314/312 (101%)	300 (96%)	14 (4%)	27	8
1	B	312/312 (100%)	280 (90%)	32 (10%)	7	1
All	All	626/624 (100%)	580 (93%)	46 (7%)	14	2

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	99	LEU
1	A	100	ASN
1	A	112	MET
1	A	160	SER
1	A	199	LYS
1	A	227[A]	ASP
1	A	227[B]	ASP
1	A	229	ASP
1	A	230	TYR
1	A	238	GLN
1	A	245	GLU
1	A	253	LYS
1	A	329	GLN
1	B	83	ILE
1	B	92	ILE
1	B	106	ARG
1	B	112	MET
1	B	114	ARG
1	B	133	ARG
1	B	136	ASP
1	B	138	GLU
1	B	139	SER
1	B	140	LEU
1	B	142	ARG
1	B	143	GLU
1	B	155	LYS
1	B	157	VAL
1	B	159	SER
1	B	161	SER
1	B	163	LYS
1	B	165	GLN
1	B	174	LEU
1	B	182	GLN
1	B	191	ARG
1	B	193	ILE
1	B	199	LYS
1	B	229	ASP
1	B	230	TYR
1	B	253	LYS
1	B	263	LEU
1	B	271	CYS
1	B	297	LEU

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Mol	Chain	Res	Type
1	B	307	PHE
1	B	330	LEU
1	B	372	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	165	GLN
1	A	183	GLN
1	A	225	GLN
1	A	248	GLN
1	B	113	ASN
1	B	176	GLN
1	B	182	GLN
1	B	248	GLN
1	B	329	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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	$\# Z > 2$
6	GAR	B	411	-	17,18,18	0.78	0	21,26,26	1.15	2 (9%)
6	GAR	A	410	-	17,18,18	0.98	1 (5%)	21,26,26	1.37	3 (14%)
3	ACT	B	961	-	1,3,3	0.09	0	0,3,3	0.00	-
5	ANP	A	400	2	29,33,33	1.32	4 (13%)	31,52,52	1.82	6 (19%)
3	ACT	A	960	-	1,3,3	0.55	0	0,3,3	0.00	-
7	MPO	A	950	-	13,13,13	1.76	2 (15%)	17,17,17	1.71	5 (29%)
5	ANP	B	1003	2	29,33,33	1.38	6 (20%)	31,52,52	2.11	6 (19%)

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
6	GAR	B	411	-	-	0/12/28/28	0/1/1/1
7	MPO	A	950	-	-	1/7/15/15	0/1/1/1
5	ANP	A	400	2	-	2/14/38/38	0/3/3/3
5	ANP	B	1003	2	-	8/14/38/38	0/3/3/3
6	GAR	A	410	-	-	1/12/28/28	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	950	MPO	C3-N1	4.54	1.57	1.47
5	A	400	ANP	PB-O2B	-3.43	1.47	1.56
5	B	1003	ANP	PB-O1B	3.14	1.51	1.46
7	A	950	MPO	C1-S1	3.10	1.81	1.77
5	B	1003	ANP	PG-O1G	3.01	1.50	1.46
6	A	410	GAR	O4-C3	-2.96	1.38	1.43
5	A	400	ANP	PG-O1G	2.64	1.50	1.46
5	B	1003	ANP	C6-N6	-2.52	1.24	1.34
5	B	1003	ANP	PB-O2B	-2.42	1.50	1.56
5	B	1003	ANP	PG-O2G	-2.32	1.50	1.56
5	B	1003	ANP	O4'-C1'	-2.27	1.37	1.41
5	A	400	ANP	C6-N6	-2.04	1.26	1.34
5	A	400	ANP	C2-N1	2.01	1.37	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1003	ANP	C5-C6-N6	8.34	133.02	120.35
5	A	400	ANP	C5-C6-N6	5.09	128.09	120.35
5	A	400	ANP	O1G-PG-N3B	-4.49	105.16	111.77
5	A	400	ANP	C5-C6-N1	-3.89	111.53	120.35
5	B	1003	ANP	C2-N1-C6	3.72	125.12	118.75
7	A	950	MPO	O1-S1-C1	3.61	111.26	106.92
6	A	410	GAR	O17-P15-O12	3.60	116.31	106.73
5	B	1003	ANP	C5-C6-N1	-3.48	112.46	120.35
5	A	400	ANP	C2-N1-C6	3.08	124.03	118.75
5	A	400	ANP	O2B-PB-O1B	3.08	116.37	109.92
7	A	950	MPO	C2-C3-N1	-2.87	106.60	113.84
5	B	1003	ANP	N3-C2-N1	-2.78	124.33	128.68
6	B	411	GAR	C10-C5-C1	2.76	125.52	115.18
7	A	950	MPO	C2-C1-S1	-2.73	109.06	113.25
5	A	400	ANP	N3-C2-N1	-2.71	124.44	128.68
7	A	950	MPO	C7-N1-C4	2.69	114.87	108.83
6	B	411	GAR	O18-P15-O17	2.61	117.60	107.64
6	A	410	GAR	C3-N19-C21	2.40	126.68	122.45
6	A	410	GAR	O4-C3-C2	2.14	108.49	106.23
5	B	1003	ANP	N6-C6-N1	-2.11	114.18	118.57
5	B	1003	ANP	O3'-C3'-C2'	2.09	118.57	111.82
7	A	950	MPO	O3-S1-C1	2.07	109.11	105.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

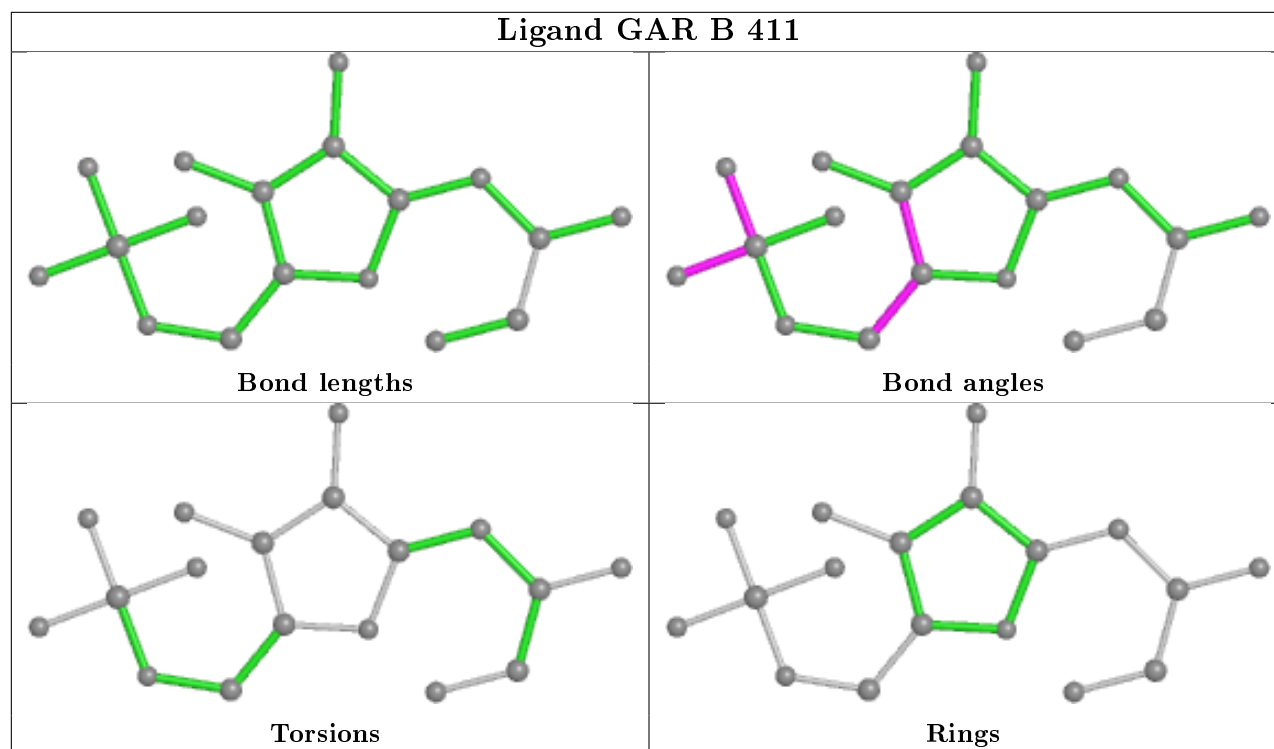
Mol	Chain	Res	Type	Atoms
5	A	400	ANP	PB-N3B-PG-O1G
5	A	400	ANP	PG-N3B-PB-O1B
5	B	1003	ANP	PB-N3B-PG-O1G
5	B	1003	ANP	PG-N3B-PB-O1B
5	B	1003	ANP	O4'-C4'-C5'-O5'
5	B	1003	ANP	C3'-C4'-C5'-O5'
6	A	410	GAR	C10-O12-P15-O16
5	B	1003	ANP	C5'-O5'-PA-O3A
5	B	1003	ANP	C5'-O5'-PA-O1A
5	B	1003	ANP	PB-O3A-PA-O1A
5	B	1003	ANP	C5'-O5'-PA-O2A
7	A	950	MPO	C1-C2-C3-N1

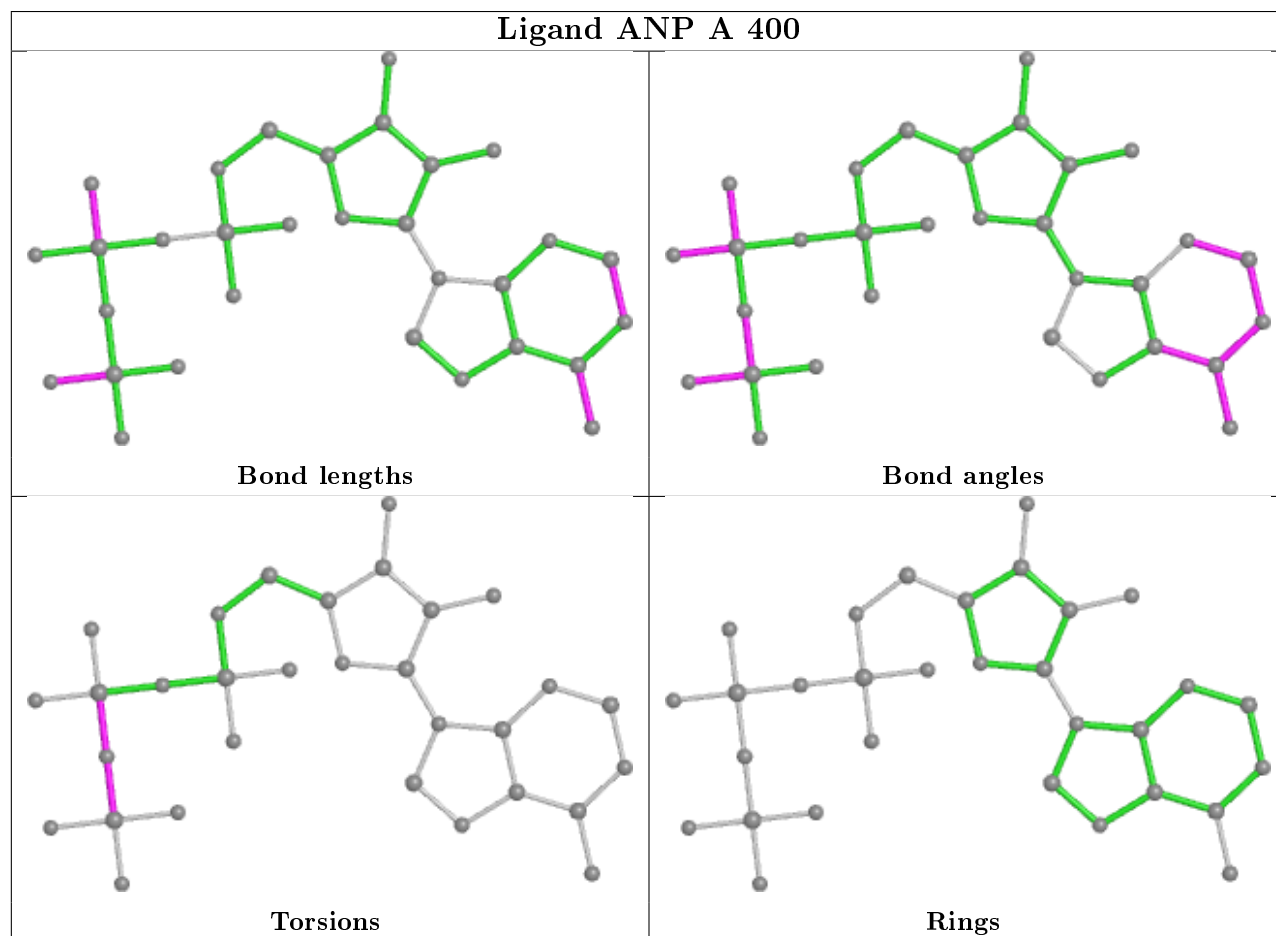
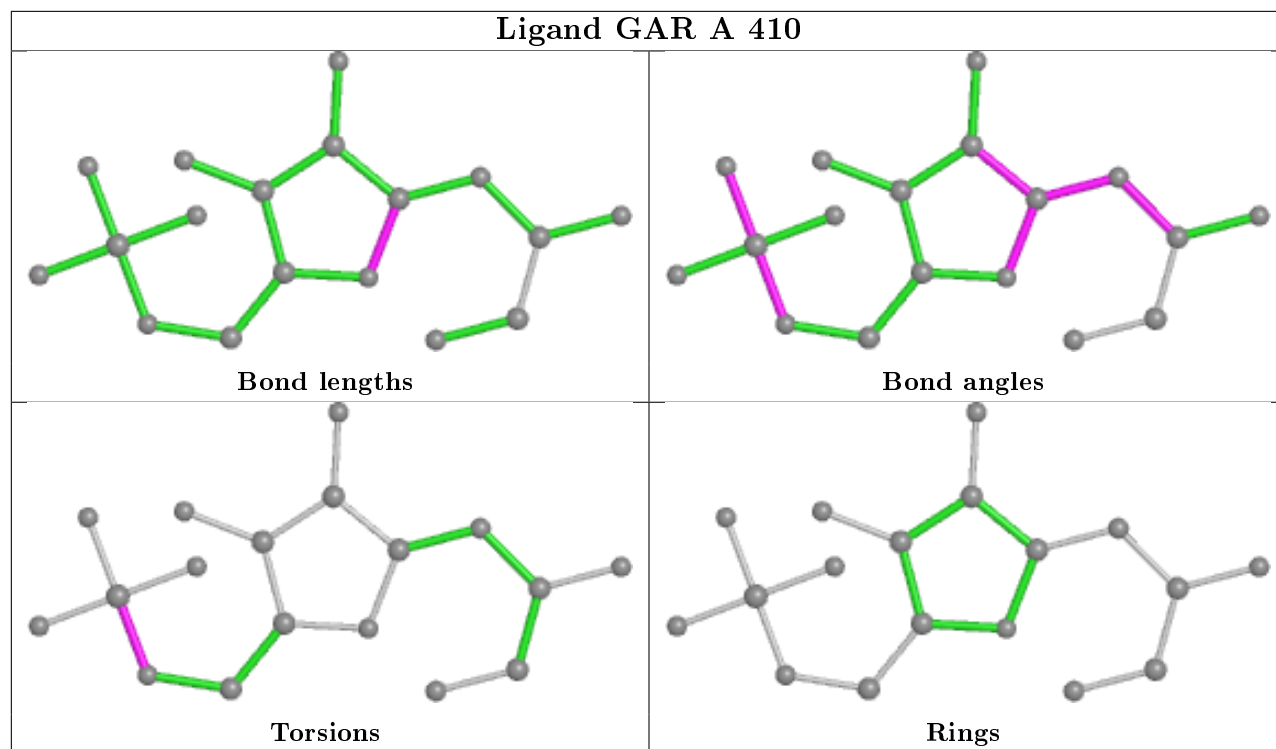
There are no ring outliers.

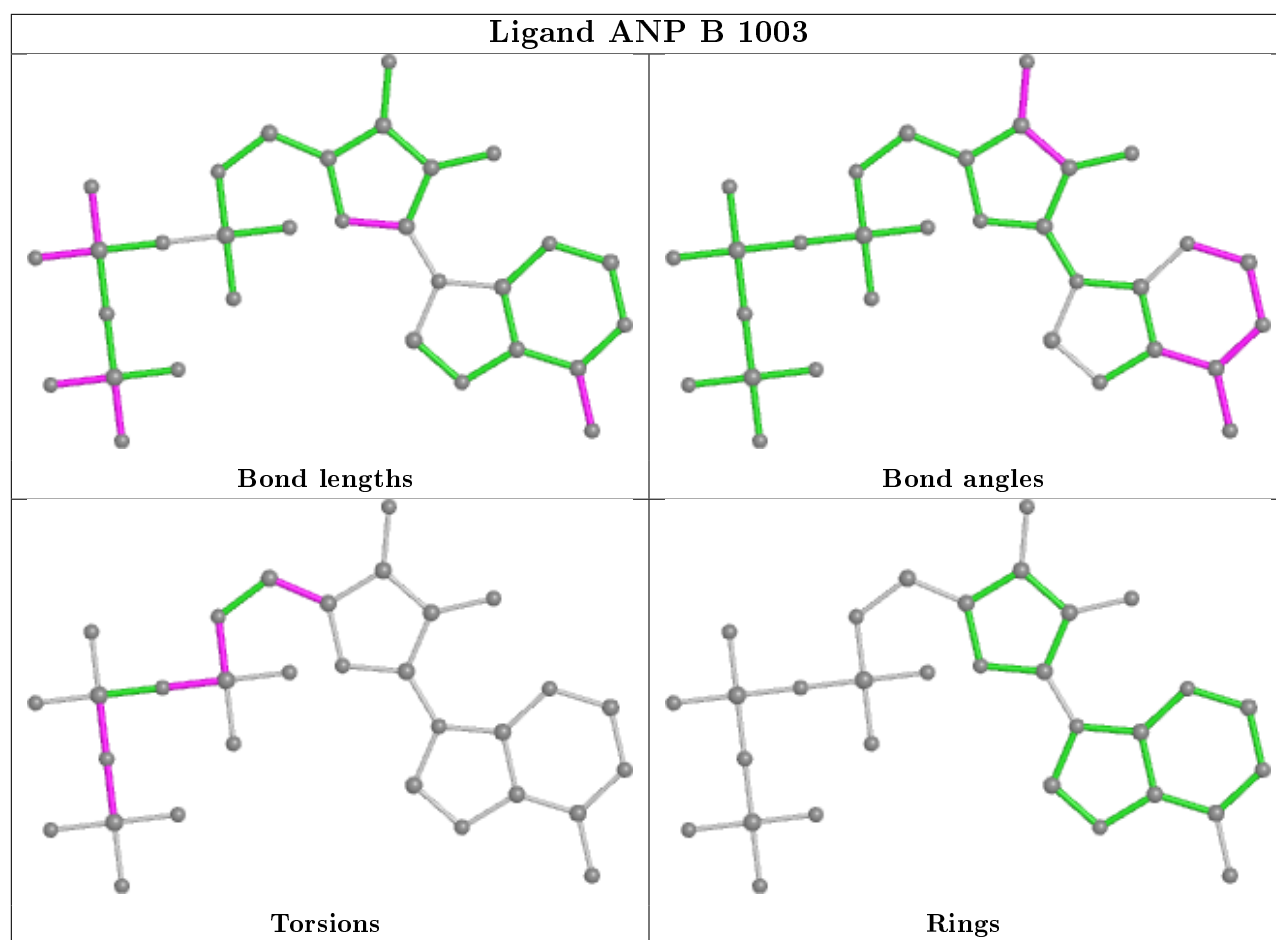
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	411	GAR	1	0
3	A	960	ACT	1	0
5	B	1003	ANP	3	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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/392 (99%)	-0.38	2 (0%) 91 93	7, 14, 45, 96	0
1	B	389/392 (99%)	0.58	61 (15%) 2 3	8, 19, 94, 100	0
All	All	778/784 (99%)	0.10	63 (8%) 12 16	7, 16, 85, 100	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	15.8
1	B	148	ILE	13.6
1	B	150	TYR	10.3
1	B	135	ALA	9.6
1	B	141	PHE	9.3
1	B	160	SER	9.0
1	B	162	GLY	8.9
1	B	159	SER	8.9
1	B	184	GLY	8.7
1	B	161	SER	8.5
1	B	192	VAL	8.4
1	B	178	TRP	8.1
1	B	176	GLN	7.8
1	B	197	VAL	7.7
1	B	187	ALA	7.6
1	B	149	GLY	7.6
1	B	145	VAL	7.4
1	B	152	CYS	7.4
1	B	144	ALA	7.3
1	B	180	TYR	6.9
1	B	154	VAL	6.8
1	B	190	GLY	6.8
1	B	183	GLN	6.7
1	B	179	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	194	VAL	6.1
1	B	142	ARG	6.0
1	B	193	ILE	5.6
1	A	187	ALA	5.5
1	B	168	ILE	5.5
1	B	137	SER	5.4
1	B	132	TYR	5.4
1	B	191	ARG	4.8
1	B	134	PHE	4.7
1	B	177	ALA	4.5
1	B	169	ARG	4.3
1	B	170	SER	4.2
1	B	136	ASP	3.6
1	B	173	GLN	3.6
1	B	174	LEU	3.6
1	B	146	ALA	3.5
1	B	156	PRO	3.4
1	B	172	GLU	3.3
1	B	165	GLN	3.2
1	B	186	ARG	3.1
1	B	138	GLU	3.0
1	B	158	MET	3.0
1	B	151	PRO	2.9
1	B	131	THR	2.8
1	B	166	THR	2.8
1	B	143	GLU	2.7
1	B	167	PHE	2.7
1	A	176	GLN	2.6
1	B	181	ALA	2.4
1	B	147	ASP	2.4
1	B	99	LEU	2.3
1	B	139	SER	2.3
1	B	185	GLY	2.3
1	B	140	LEU	2.2
1	B	133	ARG	2.1
1	B	198	VAL	2.1
1	B	199	LYS	2.1
1	B	114	ARG	2.0
1	B	196	GLY	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 [i](#)

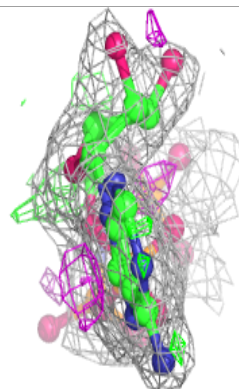
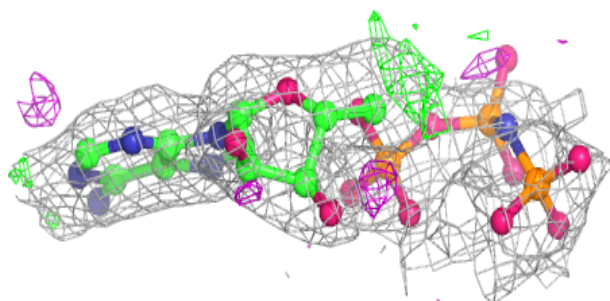
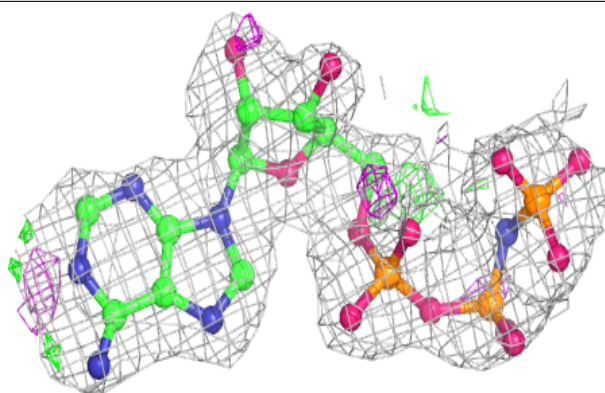
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	401	1/1	0.21	0.27	65,65,65,65	0
4	NA	B	1002	1/1	0.85	0.29	18,18,18,18	0
2	MG	B	402	1/1	0.86	0.14	65,65,65,65	0
3	ACT	B	961	4/4	0.90	0.14	39,48,53,54	0
4	NA	A	1001	1/1	0.90	0.29	13,13,13,13	0
5	ANP	B	1003	31/31	0.91	0.12	23,45,100,100	0
7	MPO	A	950	13/13	0.97	0.07	14,18,29,33	0
3	ACT	A	960	4/4	0.97	0.05	17,19,20,23	0
6	GAR	B	411	18/18	0.98	0.05	7,13,21,21	0
6	GAR	A	410	18/18	0.98	0.06	7,12,16,16	0
2	MG	A	401	1/1	0.99	0.05	15,15,15,15	0
5	ANP	A	400	31/31	0.99	0.05	7,11,17,19	0
2	MG	A	402	1/1	1.00	0.04	11,11,11,11	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.

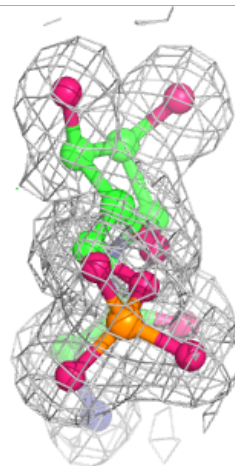
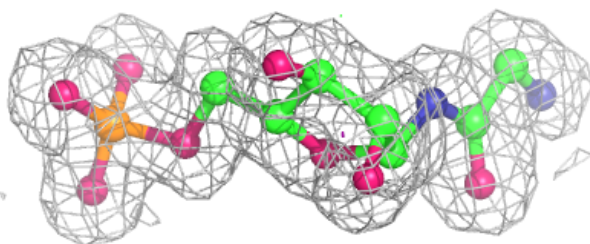
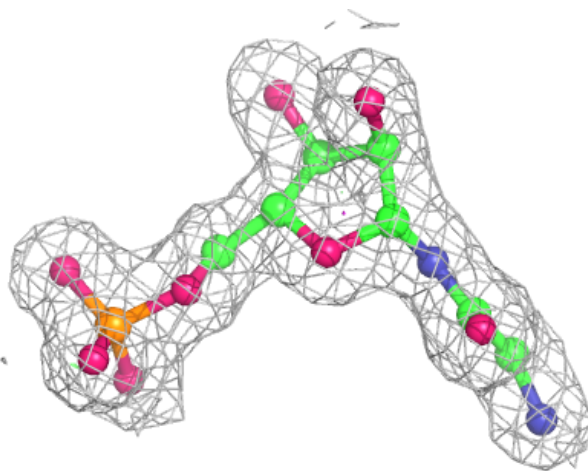
Electron density around ANP B 1003:

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



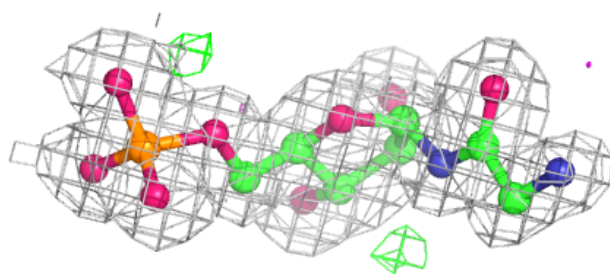
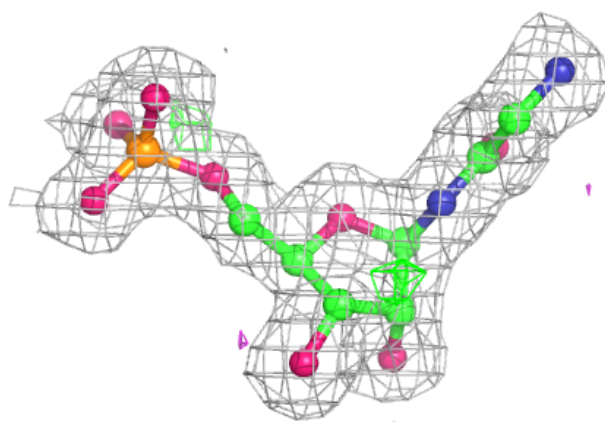
Electron density around GAR B 411:

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

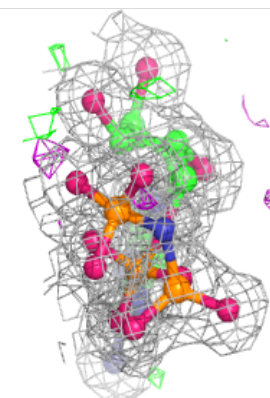
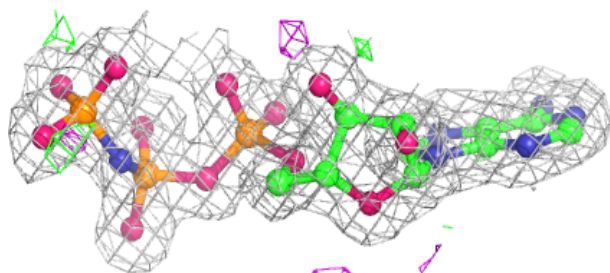
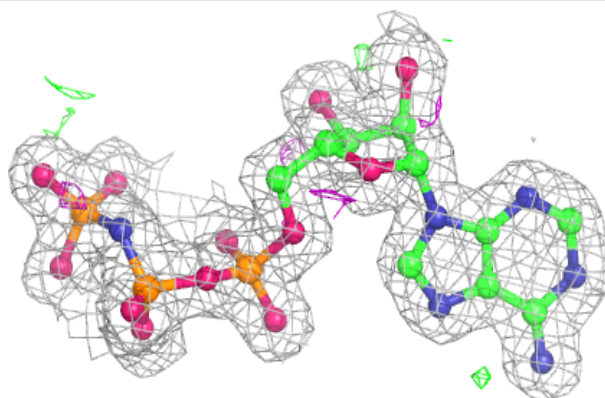


Electron density around GAR A 410:

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

**Electron density around ANP A 400:**

$2mF_o-DF_c$ (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.