



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:42 AM UTC

PDB ID : 1EZ1 / pdb_00001ez1
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

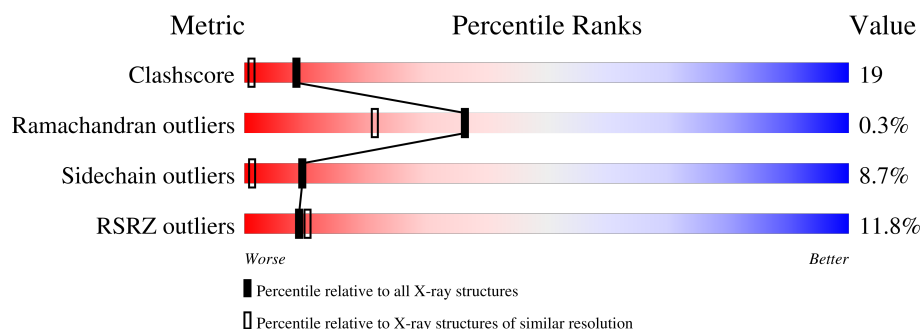
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	3% 75% 21% ..
1	B	392	20% 60% 31% 7% ..

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.

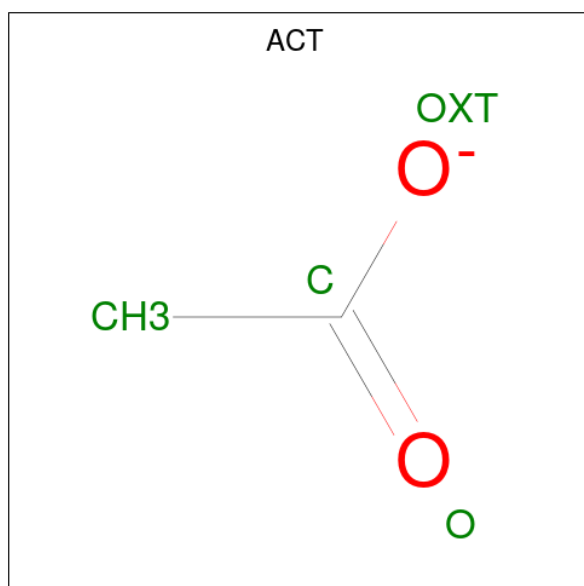
- Molecule 1 is a protein called PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE 2.

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

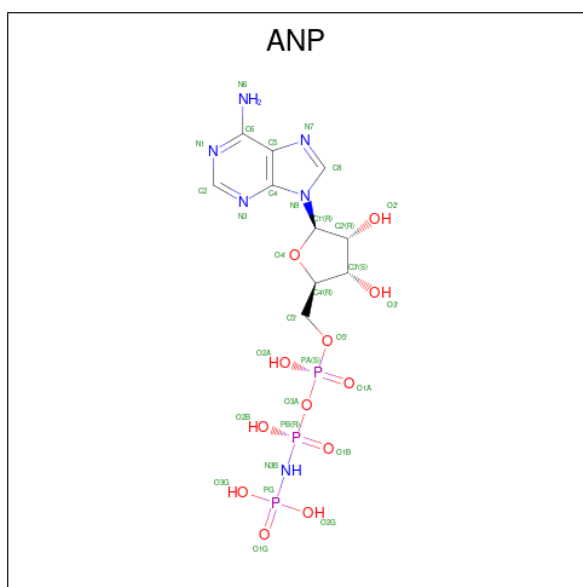


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

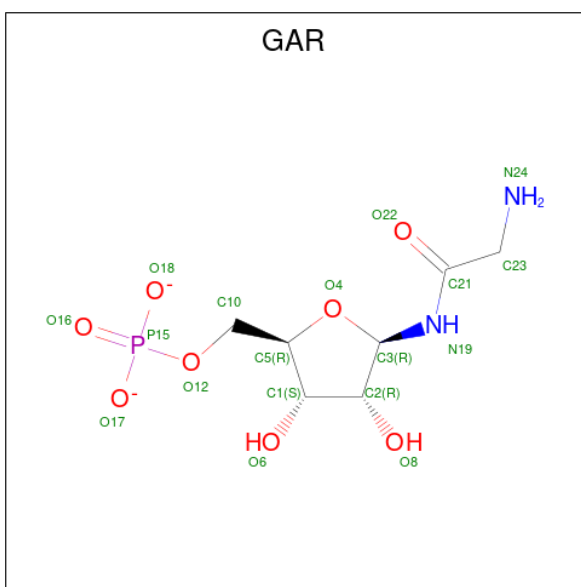
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



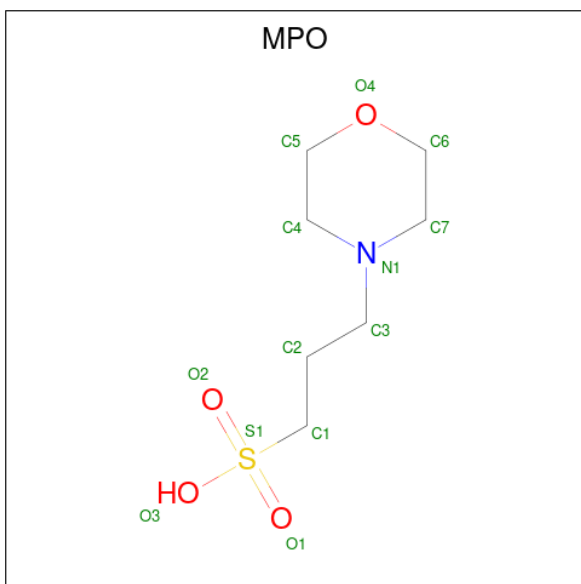
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 6 is GLYCINAMIDE RIBONUCLEOTIDE (CCD ID: GAR) (formula: $C_7H_{13}N_2O_8P$).



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 (CCD ID: MPO) (formula: C₇H₁₅NO₄S).



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

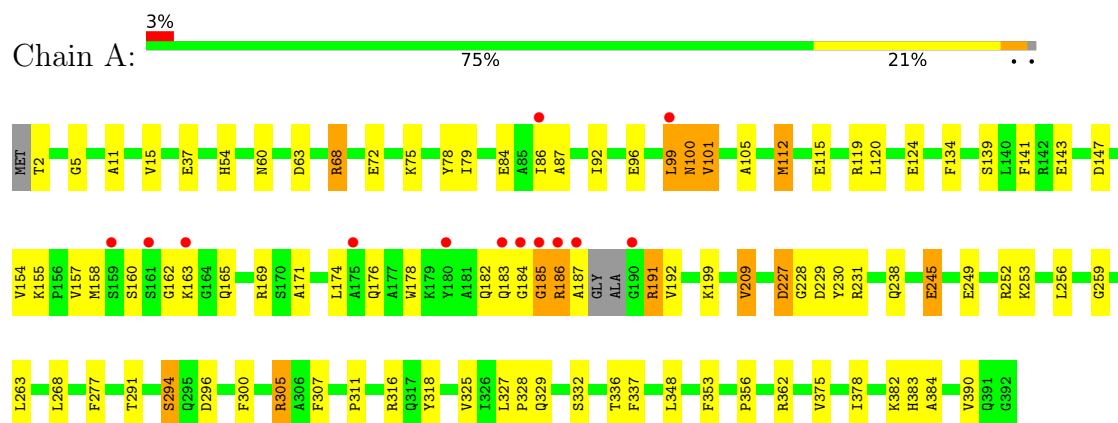
- Molecule 8 is water.

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

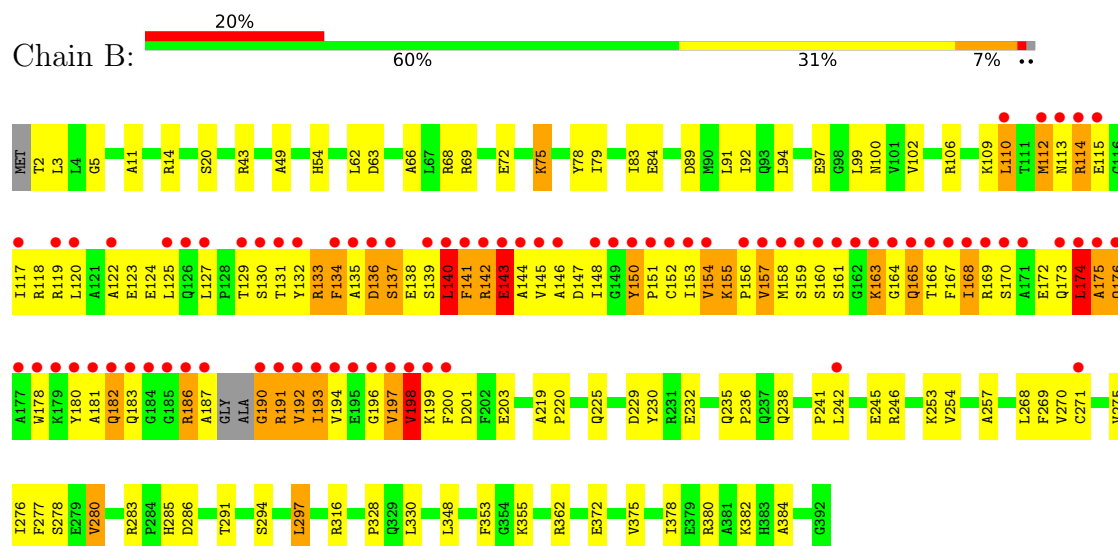
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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, α , β , γ	61.80Å 179.40Å 75.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 30.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-1.75) 97.2 (30.00-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 1.69Å)	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)	0.37 , 114.9	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, NA, ACT, GAR, 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	1.07	0/3037	1.54	26/4114 (0.6%)
1	B	1.11	5/3025 (0.2%)	1.68	42/4097 (1.0%)
All	All	1.09	5/6062 (0.1%)	1.61	68/8211 (0.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	GLY	C-N	8.14	1.43	1.33
1	B	140	LEU	C-N	7.16	1.42	1.33
1	B	141	PHE	N-CA	6.39	1.53	1.46
1	B	141	PHE	CA-CB	6.15	1.63	1.53
1	B	137	SER	N-CA	5.28	1.52	1.45

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	VAL	CA-C-N	15.67	141.96	122.37
1	B	197	VAL	C-N-CA	15.67	141.96	122.37
1	A	191	ARG	CD-NE-CZ	11.18	140.05	124.40
1	B	141	PHE	CA-CB-CG	10.96	124.76	113.80
1	B	140	LEU	CA-C-N	10.74	135.71	120.79
1	B	140	LEU	C-N-CA	10.74	135.71	120.79
1	B	197	VAL	O-C-N	9.72	133.15	122.75
1	A	353	PHE	N-CA-C	9.61	122.76	111.71
1	A	227[A]	ASP	CA-CB-CG	9.15	121.75	112.60
1	A	227[B]	ASP	CA-CB-CG	9.15	121.75	112.60
1	B	353	PHE	N-CA-C	9.11	123.66	112.54
1	B	197	VAL	N-CA-C	9.01	122.39	109.51
1	A	191	ARG	NE-CZ-NH2	8.82	127.14	119.20
1	B	140	LEU	N-CA-CB	8.55	122.40	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	HIS	CA-CB-CG	-8.01	105.79	113.80
1	B	141	PHE	N-CA-CB	7.88	121.80	109.82
1	B	190	GLY	CA-C-N	7.82	135.68	121.85
1	B	190	GLY	C-N-CA	7.82	135.68	121.85
1	B	198	VAL	N-CA-CB	-7.53	102.42	111.00
1	B	168	ILE	N-CA-C	7.28	118.61	107.99
1	A	305	ARG	CD-NE-CZ	-6.92	114.71	124.40
1	B	175	ALA	N-CA-C	-6.84	103.51	110.97
1	B	192	VAL	N-CA-C	6.65	116.93	108.82
1	B	186	ARG	O-C-N	6.46	128.75	122.03
1	B	143	GLU	N-CA-CB	6.42	119.68	110.06
1	A	185	GLY	N-CA-C	-6.34	105.13	111.85
1	A	300	PHE	CA-CB-CG	-6.33	107.47	113.80
1	A	191	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	B	198	VAL	CB-CA-C	-6.17	103.49	110.96
1	B	141	PHE	CA-C-N	6.05	129.21	120.79
1	B	141	PHE	C-N-CA	6.05	129.21	120.79
1	B	186	ARG	CA-C-N	5.97	132.45	121.70
1	B	186	ARG	C-N-CA	5.97	132.45	121.70
1	A	147	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	325	VAL	N-CA-C	5.87	117.61	109.80
1	A	294	SER	N-CA-C	5.86	120.42	113.28
1	B	102	VAL	CA-C-O	-5.81	115.72	119.15
1	A	296	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	174	LEU	N-CA-CB	5.72	120.16	110.49
1	B	245	GLU	CA-CB-CG	5.68	125.46	114.10
1	B	140	LEU	CA-C-O	-5.58	114.96	120.82
1	B	220	PRO	CB-CA-C	-5.58	104.48	111.56
1	B	141	PHE	O-C-N	5.53	128.00	122.08
1	B	134	PHE	N-CA-C	5.50	117.82	108.02
1	A	356	PRO	N-CA-C	5.47	120.95	113.84
1	B	150	TYR	CB-CA-C	5.47	116.58	108.87
1	B	285	HIS	N-CA-CB	-5.44	101.93	110.69
1	A	184	GLY	CA-C-N	-5.43	115.02	122.57
1	A	184	GLY	C-N-CA	-5.43	115.02	122.57
1	A	186	ARG	CA-C-N	5.38	131.39	121.70
1	A	186	ARG	C-N-CA	5.38	131.39	121.70
1	B	62	LEU	N-CA-C	-5.38	106.56	113.23
1	B	43	ARG	CD-NE-CZ	-5.33	116.93	124.40
1	B	150	TYR	C-N-CD	5.32	132.30	120.60
1	B	137	SER	N-CA-C	5.32	117.15	109.07
1	B	170	SER	N-CA-C	5.22	117.75	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ALA	N-CA-C	5.21	117.97	111.24
1	A	183	GLN	CA-CB-CG	-5.19	103.72	114.10
1	A	307	PHE	N-CA-CB	5.17	118.29	110.28
1	A	101	VAL	CA-C-N	-5.13	118.32	123.04
1	A	101	VAL	C-N-CA	-5.13	118.32	123.04
1	A	383	HIS	CA-CB-CG	-5.13	108.67	113.80
1	B	355	LYS	O-C-N	5.05	125.80	121.30
1	B	241	PRO	N-CA-C	-5.04	106.53	113.53
1	A	332	SER	N-CA-CB	-5.04	103.76	111.56
1	A	259	GLY	N-CA-C	5.03	119.19	112.65
1	A	229	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	130	SER	N-CA-C	-5.01	104.07	110.53

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	59	0
1	B	2972	0	2997	173	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	229	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 19.

All (229) 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:158:MET:HE3	1:A:186:ARG:HG3	1.24	1.10
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:B:152:CYS:C	1:B:153:ILE:HD12	2.02	0.83
1:B:141:PHE:CE1	1:B:145:VAL:HG21	2.13	0.83
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:232:GLU:CD	1:B:382:LYS:HD2	2.09	0.77
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:HD23	1:B:174:LEU:N	2.01	0.75
1:B:269:PHE:CE2	1:B:278:SER:HB2	2.23	0.74
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:168:ILE:HG23	1:B:173:GLN:OE1	1.89	0.72
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:173:GLN:O	1:B:176:GLN:N	2.26	0.69
1:B:201:ASP:HB2	1:B:270:VAL:O	1.92	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:HD12	1:B:153:ILE:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:158:MET:HE3	1:A:186:ARG:CG	2.13	0.67
1:A:100:ASN:C	1:A:100:ASN:HD22	2.02	0.66
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:B:173:GLN:O	1:B:176:GLN:HB2	2.00	0.61
1:B:182:GLN:HE21	1:B:182:GLN:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ILE:N	1:B:276:ILE:HD12	2.21	0.55
1:A:68:ARG:HG2	8:A:1664:HOH:O	2.06	0.55
1:A:185:GLY:C	1:A:187:ALA:H	2.13	0.54
1:B:142:ARG:HH12	1:B:174:LEU:C	2.15	0.54
1:B:137:SER:OG	1:B:140:LEU:HB2	2.08	0.54
1:B:63:ASP:HB3	1:B:66:ALA:HB3	1.90	0.54
1:B:153:ILE:CD1	1:B:197:VAL:HG23	2.38	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:20:SER:HB3	1:B:49:ALA:HB3	1.91	0.53
1:B:181:ALA:HB3	1:B:182:GLN:HE22	1.73	0.53
1:B:380:ARG:HG3	1:B:380:ARG:NH1	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:156:PRO:C	1:B:158:MET:H	2.18	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
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:N	2.69	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:191:ARG:HG3	1:B:192:VAL:N	2.24	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:99:LEU:HD13	8:B:2214:HOH:O	2.14	0.48
1:B:154:VAL:HG23	1:B:194:VAL:HG22	1.94	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:135:ALA:HB1	1:B:140:LEU:C	2.39	0.47
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.80	0.47
1:B:72:GLU:O	1:B:75:LYS:HE3	2.15	0.47
1:B:135:ALA:HB1	1:B:141:PHE:N	2.30	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:OD2	1:B:136:ASP:N	2.48	0.46
1:B:186:ARG:HD2	1:B:190:GLY:HA2	1.97	0.46
1:B:68:ARG:HH12	1:B:97:GLU:CD	2.24	0.46
1:B:72:GLU:HA	1:B:75:LYS:HE3	1.97	0.46
1:B:157:VAL:C	1:B:158:MET:HG2	2.41	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:275:VAL:C	1:B:276:ILE:HD12	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:HG3	1:B:269:PHE:CE1	2.51	0.45
1:A:100:ASN:C	1:A:100:ASN:ND2	2.73	0.45
1:B:84:GLU:O	1:B:112:MET:HE3	2.16	0.45
1:B:174:LEU:N	1:B:174:LEU:CD2	2.75	0.45
1:B:91:LEU:HD23	1:B:91:LEU:HA	1.81	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: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:203:GLU:CG	1:B:269:PHE:CD1	2.99	0.44
1:B:242:LEU:HD21	1:B:246:ARG:CZ	2.48	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:2:THR:N	3:A:960:ACT:OXT	2.52	0.42
1:A:134:PHE:HB3	1:A:191:ARG:HD3	2.01	0.42
1:B:156:PRO:HD3	1:B:164:GLY:O	2.19	0.42
1:B:125:LEU:HD11	1:B:257:ALA:HB3	1.99	0.42
1:B:131:THR:O	1:B:132:TYR:HB3	2.19	0.42
1:B:225:GLN:HE21	1:B:225:GLN:HB3	1.56	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:79:ILE:HD11	1:B:99:LEU:HD12	2.02	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:A:5:GLY:HA3	1:A:11:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:TYR:CD2	1:B:169:ARG:C	2.98	0.42
1:B:156:PRO:C	1:B:158:MET:N	2.78	0.42
1:B:181:ALA:C	1:B:182:GLN:NE2	2.77	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:HD23	1:B:94:LEU:HA	1.85	0.41
1:A:327:LEU:HD12	1:A:362:ARG:C	2.46	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:HH11	1:B:316[B]:ARG:HD3	1.64	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:131:THR:C	1:B:132:TYR:HD2	2.28	0.41
1:B:135:ALA:CB	1:B:141:PHE:HA	2.51	0.41
1:B:167:PHE:CD1	1:B:167:PHE:C	2.99	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:133:ARG:C	1:B:134:PHE:CD2	2.99	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:173:GLN:C	1:B:175:ALA:N	2.79	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

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	388/392 (99%)	380 (98%)	8 (2%)	0	100	100
1	B	386/392 (98%)	364 (94%)	20 (5%)	2 (0%)	24	11
All	All	774/784 (99%)	744 (96%)	28 (4%)	2 (0%)	36	21

All (2) Ramachandran outliers are listed below:

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

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	314/312 (101%)	298 (95%)	16 (5%)	21	5
1	B	312/312 (100%)	273 (88%)	39 (12%)	4	0
All	All	626/624 (100%)	571 (91%)	55 (9%)	9	1

All (55) 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

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Mol	Chain	Res	Type
1	A	160	SER
1	A	163	LYS
1	A	169	ARG
1	A	199	LYS
1	A	209	VAL
1	A	227[A]	ASP
1	A	227[B]	ASP
1	A	230	TYR
1	A	238	GLN
1	A	245	GLU
1	A	253	LYS
1	A	329	GLN
1	B	75	LYS
1	B	83	ILE
1	B	92	ILE
1	B	106	ARG
1	B	110	LEU
1	B	112	MET
1	B	114	ARG
1	B	120	LEU
1	B	124	GLU
1	B	127	LEU
1	B	133	ARG
1	B	136	ASP
1	B	139	SER
1	B	140	LEU
1	B	142	ARG
1	B	143	GLU
1	B	154	VAL
1	B	155	LYS
1	B	157	VAL
1	B	161	SER
1	B	163	LYS
1	B	165	GLN
1	B	172	GLU
1	B	174	LEU
1	B	182	GLN
1	B	191	ARG
1	B	193	ILE
1	B	198	VAL
1	B	199	LYS
1	B	229	ASP

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Mol	Chain	Res	Type
1	B	230	TYR
1	B	238	GLN
1	B	253	LYS
1	B	271	CYS
1	B	280	VAL
1	B	297	LEU
1	B	330	LEU
1	B	372	GLU
1	B	375	VAL

Sometimes 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	165	GLN
1	A	183	GLN
1	A	329	GLN
1	B	113	ASN
1	B	176	GLN
1	B	182	GLN
1	B	248	GLN
1	B	383	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.77	0	22,26,26	1.46	4 (18%)
6	GAR	A	410	-	17,18,18	0.95	1 (5%)	22,26,26	1.49	4 (18%)
5	ANP	A	400	2	33,33,33	1.40	5 (15%)	45,52,52	1.47	6 (13%)
3	ACT	A	960	-	3,3,3	0.79	0	3,3,3	1.20	0
7	MPO	A	950	-	13,13,13	1.79	2 (15%)	17,17,17	1.60	4 (23%)
5	ANP	B	1003	2	33,33,33	1.42	5 (15%)	45,52,52	1.41	4 (8%)
3	ACT	B	961	-	3,3,3	0.81	0	3,3,3	0.82	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
6	GAR	B	411	-	-	0/12/28/28	0/1/1/1
6	GAR	A	410	-	-	1/12/28/28	0/1/1/1
5	ANP	A	400	2	-	2/18/38/38	0/3/3/3
7	MPO	A	950	-	-	0/7/15/15	0/1/1/1
5	ANP	B	1003	2	-	7/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	950	MPO	C3-N1	4.59	1.57	1.47
5	B	1003	ANP	C6-N6	-3.72	1.24	1.34
5	A	400	ANP	PB-O2B	-3.49	1.47	1.56
5	B	1003	ANP	PB-O1B	3.27	1.51	1.46
5	B	1003	ANP	PG-O1G	3.13	1.50	1.46
7	A	950	MPO	C1-S1	3.08	1.81	1.77
5	A	400	ANP	C6-N6	-3.04	1.26	1.34
6	A	410	GAR	O4-C3	-2.78	1.38	1.43
5	A	400	ANP	PG-O1G	2.74	1.50	1.46
5	B	1003	ANP	PB-O2B	-2.47	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1003	ANP	PG-O2G	-2.37	1.50	1.56
5	A	400	ANP	C2-N3	-2.25	1.29	1.33
5	A	400	ANP	C2-N1	2.09	1.37	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	400	ANP	O1G-PG-N3B	-4.49	105.16	111.77
5	B	1003	ANP	C5-C6-N6	3.93	133.02	123.29
5	B	1003	ANP	C2-N1-C6	3.89	125.12	118.73
6	A	410	GAR	O17-P15-O12	3.70	116.31	106.67
6	B	411	GAR	O4-C3-N19	-3.53	106.23	110.22
5	A	400	ANP	C2-N1-C6	3.22	124.03	118.73
5	A	400	ANP	O2B-PB-O1B	3.03	116.37	109.87
7	A	950	MPO	O1-S1-C1	3.00	111.26	106.73
6	B	411	GAR	C10-C5-C1	2.86	125.52	115.21
5	B	1003	ANP	N3-C2-N1	-2.81	124.33	128.58
7	A	950	MPO	C7-N1-C4	2.80	114.87	108.84
5	A	400	ANP	N3-C2-N1	-2.74	124.44	128.58
7	A	950	MPO	C2-C1-S1	-2.73	109.06	113.25
6	B	411	GAR	C2-C3-N19	-2.65	108.68	112.02
6	B	411	GAR	O18-P15-O17	2.61	117.60	107.80
7	A	950	MPO	C2-C3-N1	-2.61	106.60	113.93
6	A	410	GAR	O4-C3-N19	-2.50	107.39	110.22
5	A	400	ANP	C6-C5-C4	2.48	120.56	117.18
5	A	400	ANP	C5-C6-N1	-2.35	111.53	117.51
6	A	410	GAR	C3-N19-C21	2.34	126.68	122.54
6	A	410	GAR	O4-C3-C2	2.12	108.49	106.29
5	B	1003	ANP	O3'-C3'-C2'	2.11	118.57	111.82

There are no chirality outliers.

All (10) 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'
6	A	410	GAR	C10-O12-P15-O16
5	B	1003	ANP	C3'-C4'-C5'-O5'
5	B	1003	ANP	PB-O3A-PA-O1A

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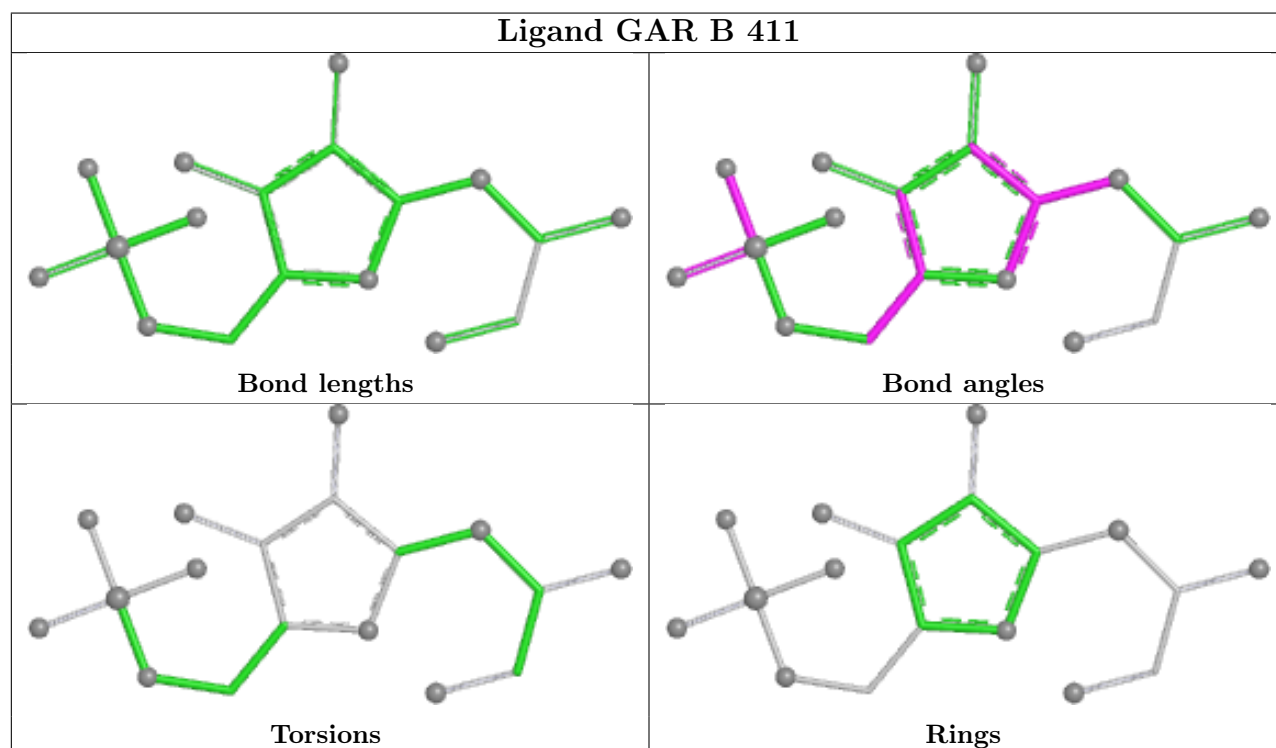
Mol	Chain	Res	Type	Atoms
5	B	1003	ANP	C5'-O5'-PA-O1A
5	B	1003	ANP	C5'-O5'-PA-O3A

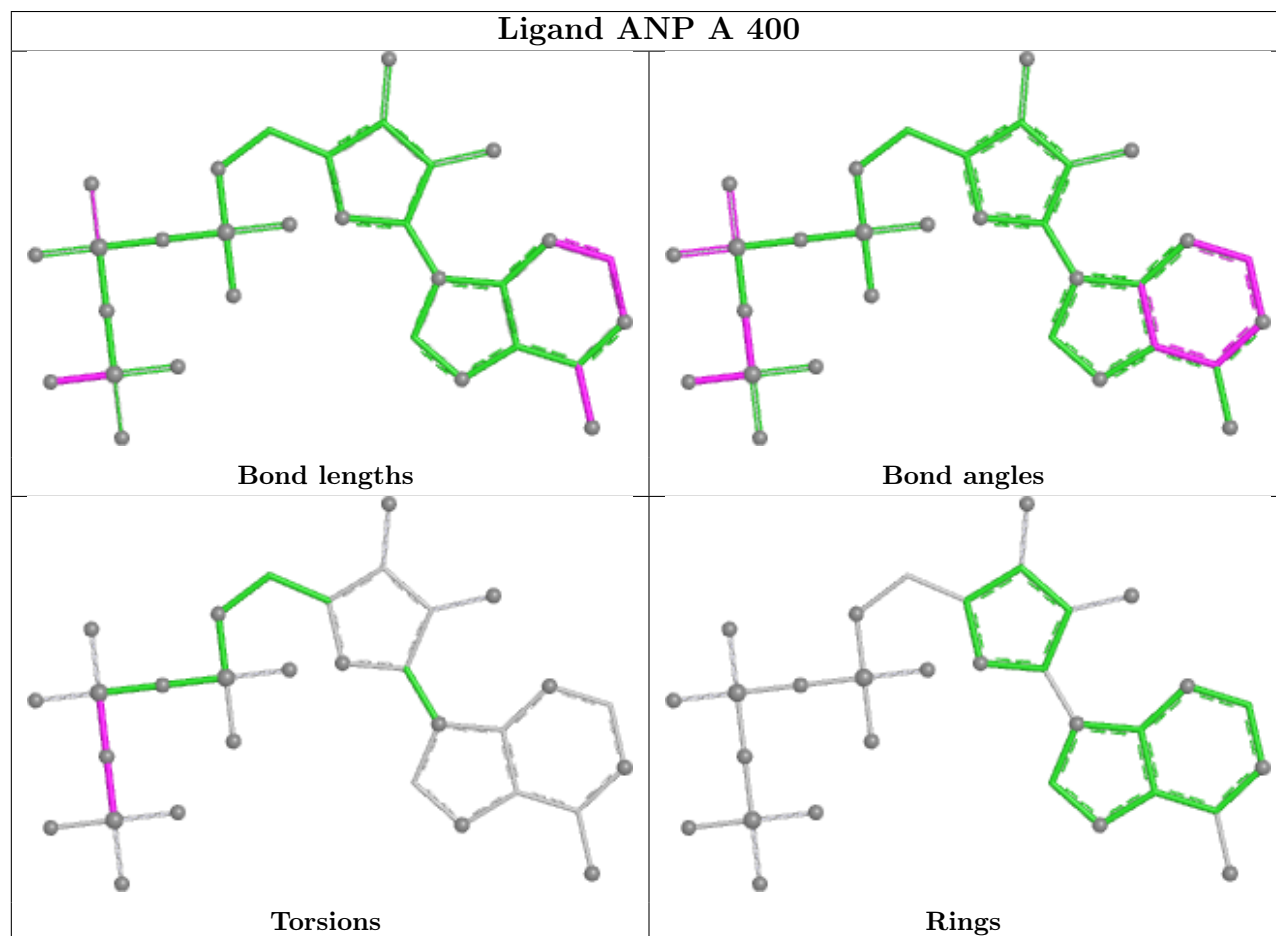
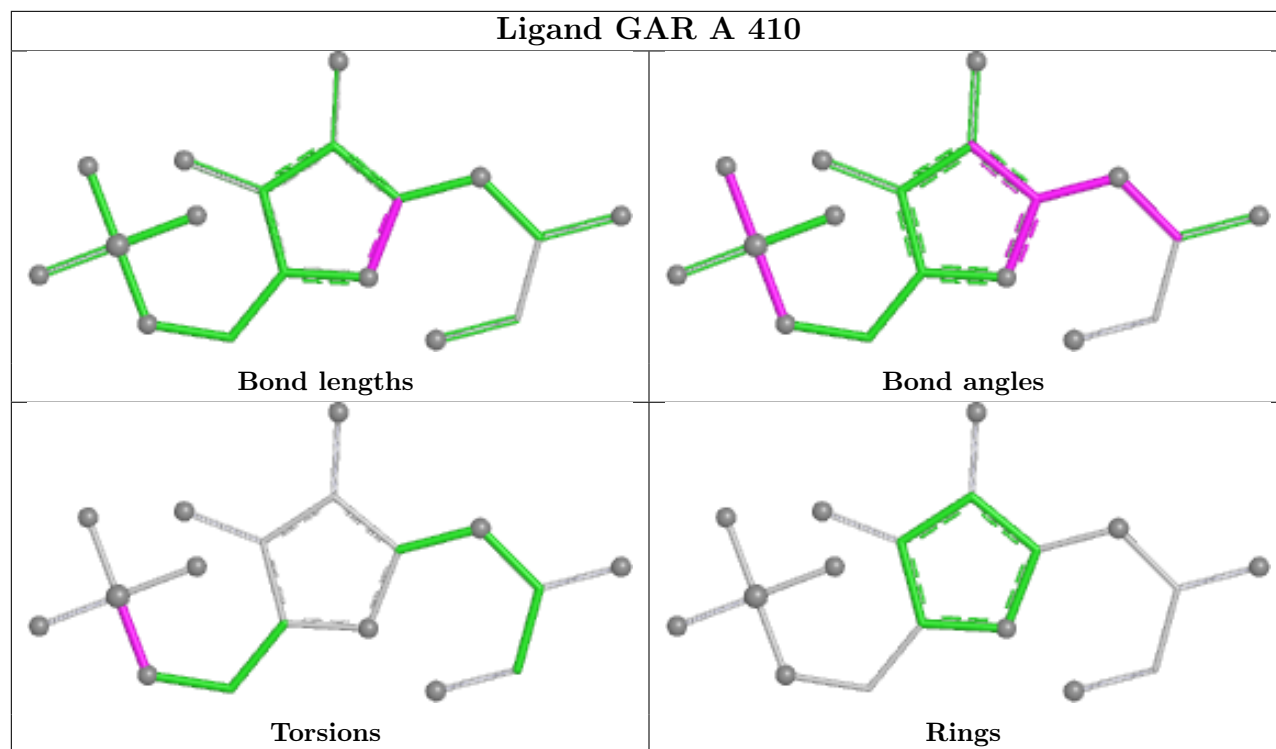
There are no ring outliers.

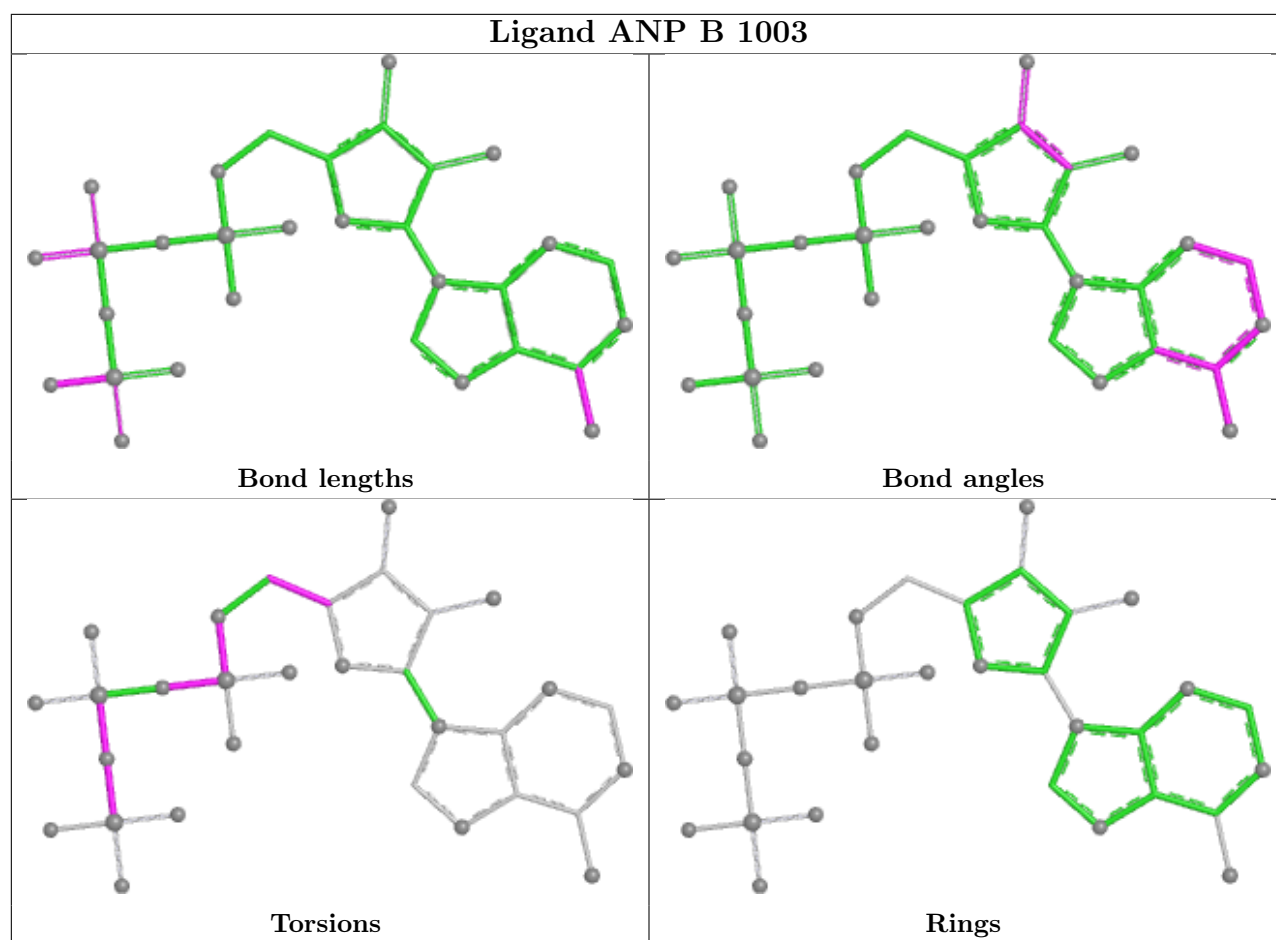
3 monomers are involved in 5 short contacts:

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%)	-0.26	13 (3%)	49 55	7, 14, 45, 96	3 (0%)
1	B	389/392 (99%)	0.65	79 (20%)	3 3	8, 19, 94, 100	1 (0%)
All	All	778/784 (99%)	0.20	92 (11%)	9 10	7, 16, 85, 100	4 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	VAL	7.9
1	B	192	VAL	7.8
1	B	197	VAL	7.8
1	B	175	ALA	6.7
1	B	135	ALA	6.4
1	B	154	VAL	6.3
1	B	193	ILE	6.3
1	B	141	PHE	6.1
1	B	162	GLY	6.1
1	B	152	CYS	6.1
1	B	148	ILE	5.6
1	A	187	ALA	5.6
1	B	144	ALA	5.2
1	B	131	THR	5.2
1	B	178	TRP	4.9
1	B	190	GLY	4.9
1	B	166	THR	4.8
1	B	187	ALA	4.6
1	B	145	VAL	4.6
1	B	181	ALA	4.6
1	B	132	TYR	4.5
1	B	184	GLY	4.5
1	B	161	SER	4.5
1	B	150	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	160	SER	4.5
1	B	177	ALA	4.4
1	B	149	GLY	4.4
1	B	185	GLY	4.2
1	B	168	ILE	4.2
1	B	156	PRO	4.1
1	A	161	SER	4.1
1	A	185	GLY	4.0
1	B	180	TYR	4.0
1	B	134	PHE	4.0
1	B	200	PHE	4.0
1	B	176	GLN	3.9
1	B	174	LEU	3.9
1	B	157	VAL	3.9
1	B	198	VAL	3.8
1	B	191	ARG	3.8
1	B	146	ALA	3.7
1	B	159	SER	3.6
1	B	167	PHE	3.5
1	B	195	GLU	3.4
1	B	136	ASP	3.4
1	B	196	GLY	3.3
1	B	137	SER	3.3
1	B	164	GLY	3.3
1	B	169	ARG	3.3
1	A	184	GLY	3.2
1	A	186	ARG	3.2
1	B	127	LEU	3.2
1	B	114	ARG	3.2
1	B	158	MET	3.1
1	B	271	CYS	3.1
1	B	171	ALA	3.1
1	B	151	PRO	3.0
1	B	140	LEU	3.0
1	B	170	SER	3.0
1	B	139	SER	3.0
1	B	142	ARG	2.9
1	B	143	GLU	2.9
1	B	199	LYS	2.9
1	B	125	LEU	2.8
1	B	153	ILE	2.8
1	A	190	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	175	ALA	2.8
1	B	130	SER	2.8
1	B	242	LEU	2.7
1	A	86	ILE	2.7
1	B	122	ALA	2.6
1	B	163	LYS	2.6
1	B	120	LEU	2.6
1	B	186	ARG	2.6
1	B	182	GLN	2.6
1	B	179	LYS	2.5
1	B	129	THR	2.5
1	B	183	GLN	2.4
1	B	117	ILE	2.4
1	A	163	LYS	2.3
1	B	119	ARG	2.3
1	B	173	GLN	2.2
1	A	183	GLN	2.2
1	B	126	GLN	2.2
1	B	165	GLN	2.2
1	A	159	SER	2.2
1	B	115	GLU	2.1
1	B	113	ASN	2.1
1	B	110	LEU	2.1
1	A	99	LEU	2.1
1	A	180	TYR	2.1
1	B	112	MET	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](#)

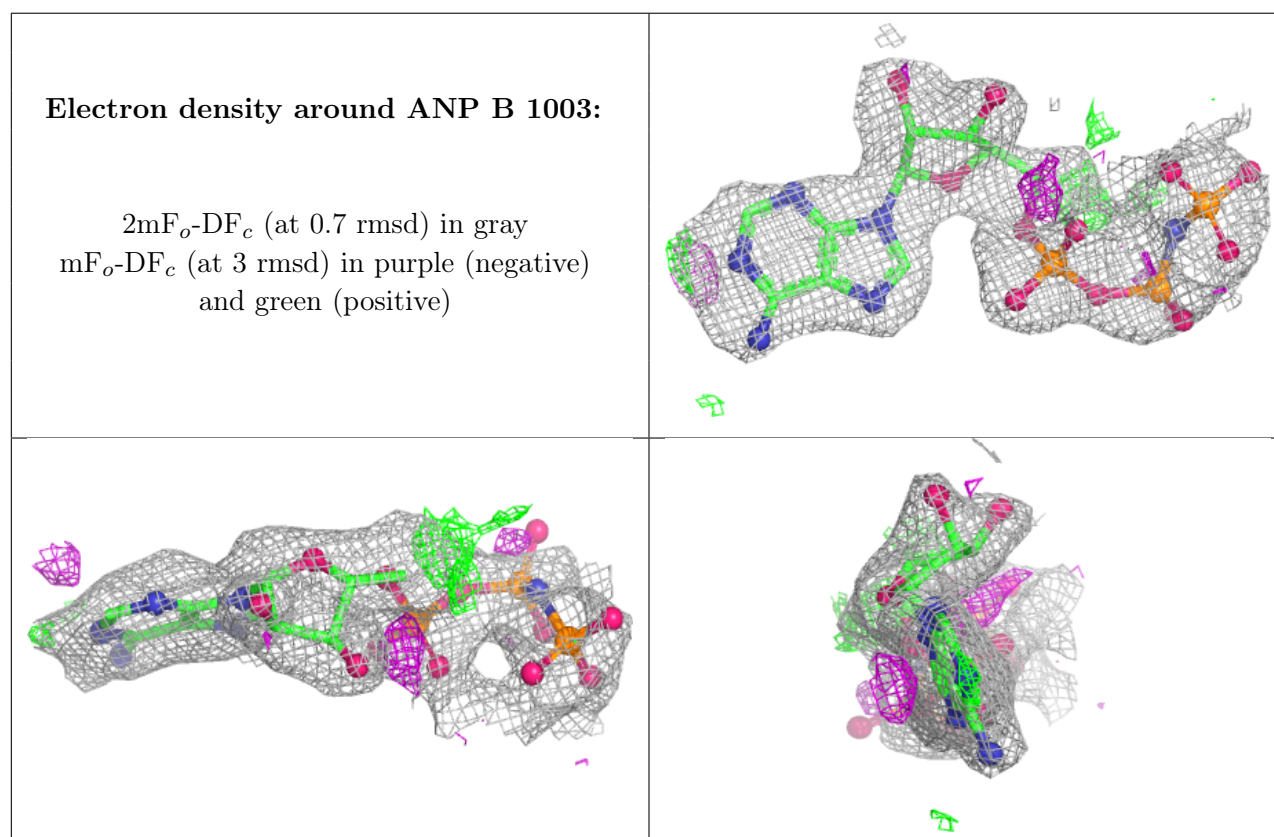
There are no oligosaccharides in this entry.

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.

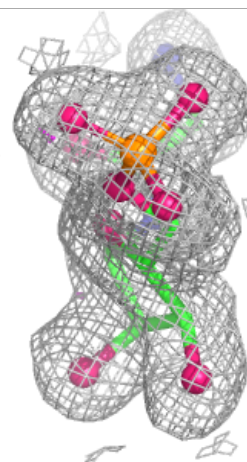
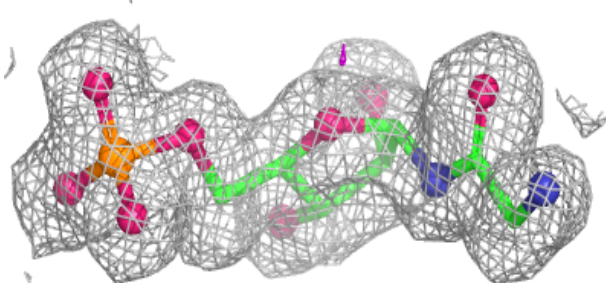
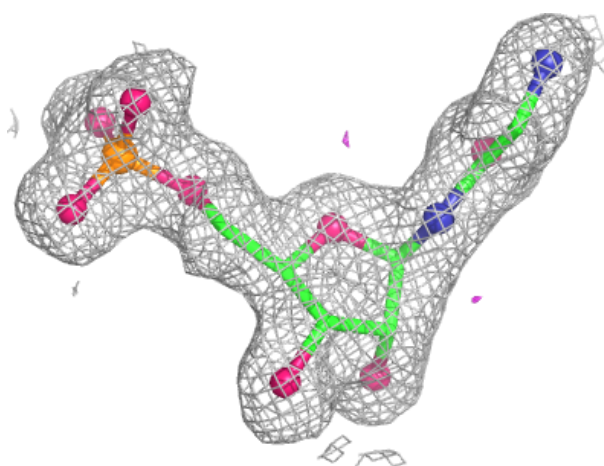
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	401	1/1	0.61	0.16	65,65,65,65	0
3	ACT	B	961	4/4	0.84	0.12	39,48,53,54	0
2	MG	B	402	1/1	0.85	0.15	65,65,65,65	0
5	ANP	B	1003	31/31	0.85	0.12	23,45,100,100	0
4	NA	B	1002	1/1	0.87	0.23	18,18,18,18	0
4	NA	A	1001	1/1	0.88	0.26	13,13,13,13	0
3	ACT	A	960	4/4	0.96	0.05	17,19,20,23	0
7	MPO	A	950	13/13	0.97	0.07	14,18,29,33	0
6	GAR	B	411	18/18	0.98	0.04	7,13,21,21	0
6	GAR	A	410	18/18	0.98	0.04	7,12,16,16	0
2	MG	A	402	1/1	0.99	0.05	11,11,11,11	0
5	ANP	A	400	31/31	0.99	0.04	7,11,17,19	0
2	MG	A	401	1/1	0.99	0.03	15,15,15,15	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.



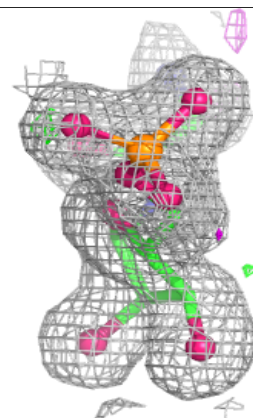
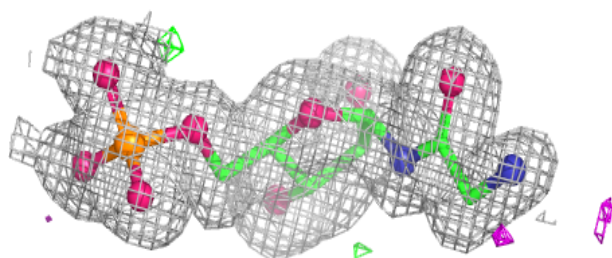
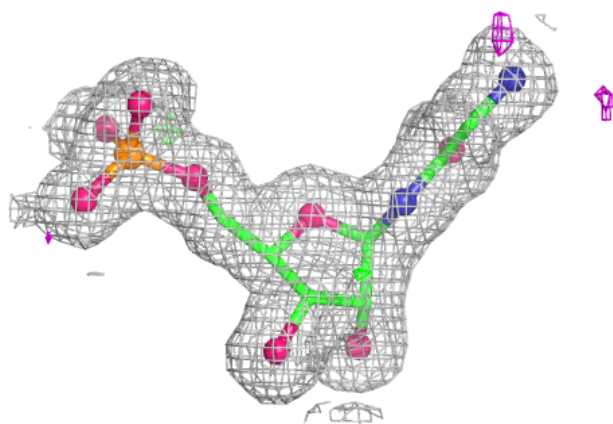
Electron density around GAR B 411:

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

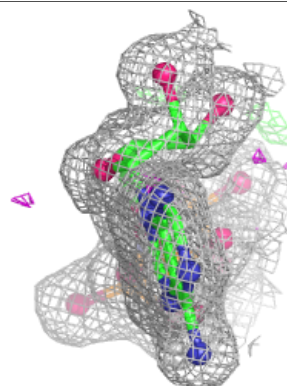
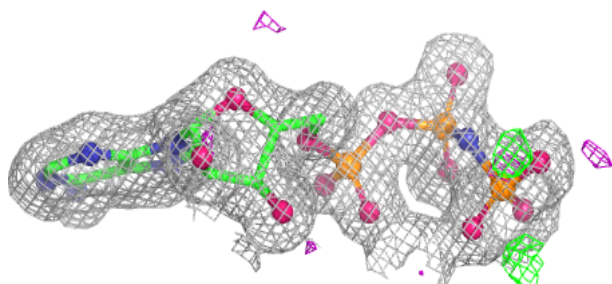
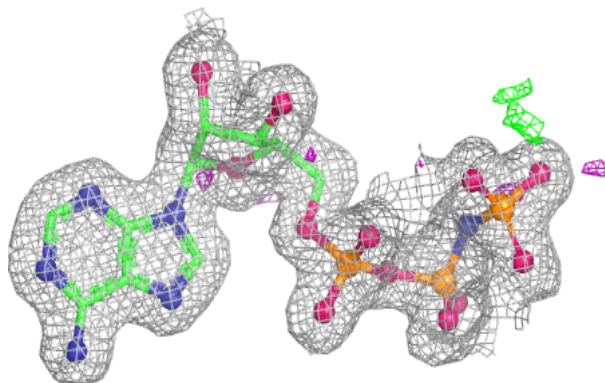


Electron density around GAR A 410:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.