



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:09 AM UTC

PDB ID : 3SGI / pdb_00003sgi
Title : Crystal structure of DNA ligase A BRCT domain deleted mutant of Mycobacterium tuberculosis
Authors : Kukshal, V.; Ravishankar, R.
Deposited on : 2011-06-15
Resolution : 3.50 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

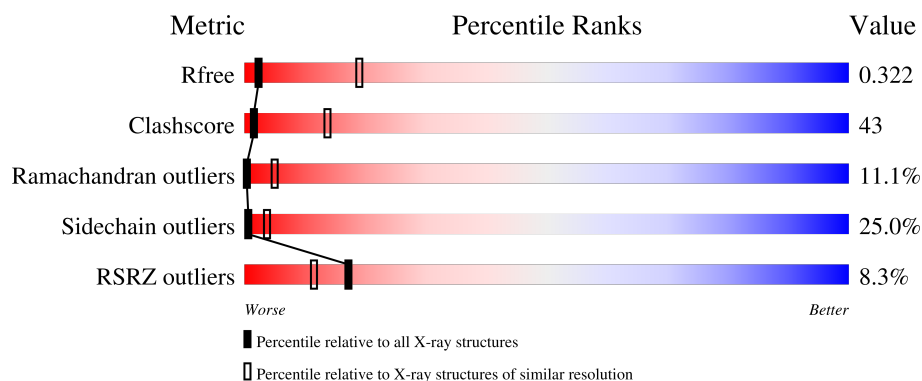
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	615	6% 25% 27% 13% • 34%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3221 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.

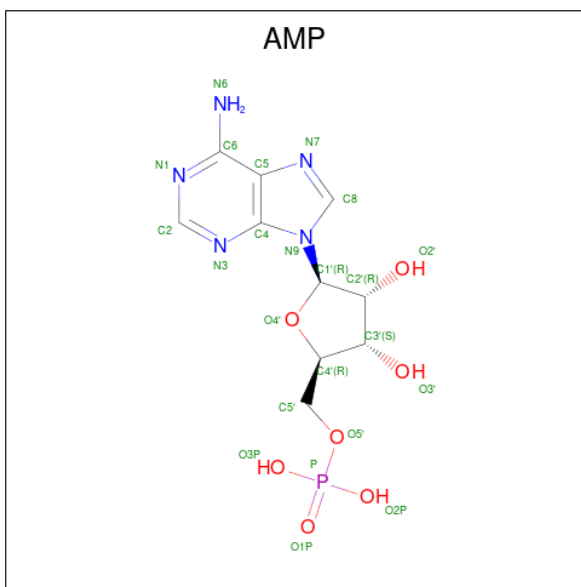
- Molecule 1 is a protein called DNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3176	1993	578	599	6			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP P63973
A	606	GLY	-	expression tag	UNP P63973
A	607	SER	-	expression tag	UNP P63973
A	608	ARG	-	expression tag	UNP P63973
A	609	SER	-	expression tag	UNP P63973
A	610	HIS	-	expression tag	UNP P63973
A	611	HIS	-	expression tag	UNP P63973
A	612	HIS	-	expression tag	UNP P63973
A	613	HIS	-	expression tag	UNP P63973
A	614	HIS	-	expression tag	UNP P63973
A	615	HIS	-	expression tag	UNP P63973

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

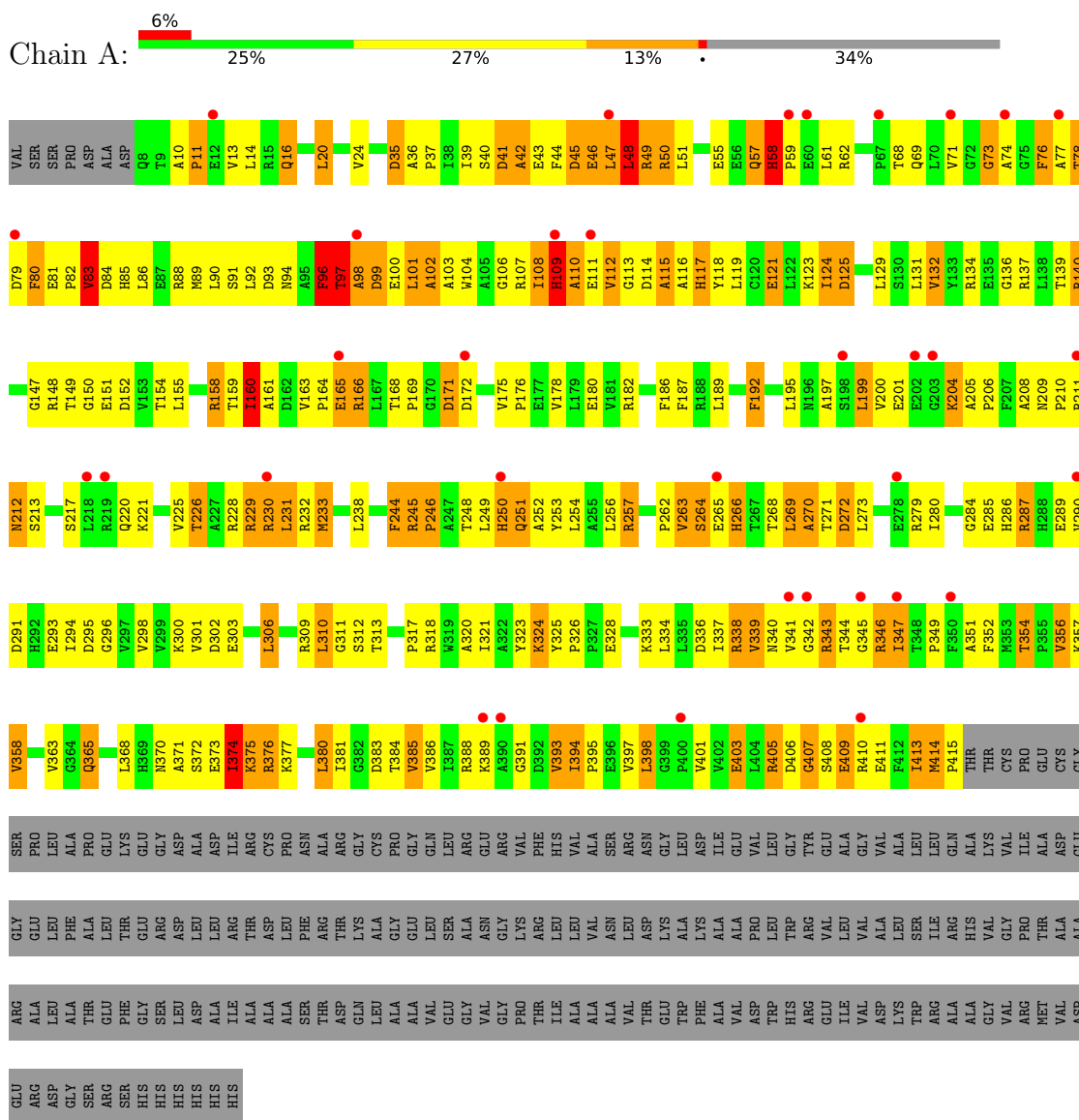
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		

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: DNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.44Å 99.56Å 144.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 3.50 49.78 – 3.50	Depositor EDS
% Data completeness (in resolution range)	89.3 (49.78-3.50) 89.3 (49.78-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.311 , 0.322 0.309 , 0.322	Depositor DCC
R_{free} test set	435 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 94.1	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	0.78	EDS
Total number of atoms	3221	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: AMP

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	0.72	1/3243 (0.0%)	1.15	21/4411 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	LYS	C-O	-5.49	1.17	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	HIS	CA-C-N	7.65	127.37	119.56
1	A	58	HIS	C-N-CA	7.65	127.37	119.56
1	A	250	HIS	N-CA-C	6.86	125.42	110.80
1	A	354	THR	CA-C-N	6.55	128.03	119.84
1	A	354	THR	C-N-CA	6.55	128.03	119.84
1	A	97	THR	N-CA-C	6.29	121.69	111.37
1	A	410	ARG	N-CA-C	6.28	117.41	108.74
1	A	40	SER	N-CA-C	6.20	118.04	111.28
1	A	48	LEU	CA-C-N	6.11	132.69	121.70
1	A	48	LEU	C-N-CA	6.11	132.69	121.70
1	A	97	THR	CA-C-N	5.81	132.16	121.70
1	A	97	THR	C-N-CA	5.81	132.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	PHE	N-CA-C	-5.67	105.01	111.14
1	A	343	ARG	N-CA-C	5.67	116.54	108.54
1	A	39	ILE	N-CA-C	5.41	116.64	108.96
1	A	250	HIS	CA-C-N	5.32	131.27	121.70
1	A	250	HIS	C-N-CA	5.32	131.27	121.70
1	A	356	VAL	N-CA-C	5.17	114.67	108.06
1	A	48	LEU	N-CA-C	5.08	121.62	110.80
1	A	76	PHE	N-CA-C	5.08	117.46	110.35
1	A	339	VAL	N-CA-C	5.08	114.73	108.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	ASP	Peptide
1	A	96	PHE	Peptide

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	3176	0	3117	269	1
2	A	22	0	12	2	0
3	A	23	0	0	2	0
All	All	3221	0	3129	270	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (270) 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:48:LEU:N	1:A:49:ARG:HB3	1.35	1.39
1:A:248:THR:OG1	1:A:251:GLN:HG3	1.44	1.16
1:A:48:LEU:H	1:A:49:ARG:CB	1.58	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:HG3	1:A:50:ARG:H	1.07	1.13
1:A:269:LEU:HA	1:A:270:ALA:HB3	1.24	1.12
1:A:346:ARG:HH21	1:A:346:ARG:HG2	1.12	1.12
1:A:80:PHE:HB2	1:A:151:GLU:HB3	1.25	1.12
1:A:46:GLU:HA	1:A:49:ARG:HD2	1.29	1.09
1:A:97:THR:HG23	1:A:98:ALA:HB3	1.32	1.07
1:A:160:ILE:HB	1:A:161:ALA:HA	1.08	1.06
1:A:264:SER:CB	1:A:265:GLU:HA	1.86	1.03
1:A:160:ILE:CB	1:A:161:ALA:HA	1.88	1.03
1:A:49:ARG:CG	1:A:50:ARG:H	1.72	1.03
1:A:264:SER:OG	1:A:265:GLU:HA	1.60	1.02
1:A:265:GLU:HB2	1:A:266:HIS:HB2	1.46	0.97
1:A:284:GLY:H	1:A:287:ARG:HB3	1.27	0.96
1:A:269:LEU:HA	1:A:270:ALA:CB	1.95	0.96
1:A:248:THR:OG1	1:A:251:GLN:CG	2.15	0.95
1:A:77:ALA:N	1:A:78:THR:HA	1.81	0.94
1:A:45:ASP:HB3	1:A:46:GLU:O	1.67	0.94
1:A:195:LEU:HD11	1:A:229:ARG:HD2	1.50	0.92
1:A:264:SER:HB3	1:A:265:GLU:HG3	1.51	0.91
1:A:339:VAL:HG12	1:A:340:ASN:H	1.35	0.91
1:A:49:ARG:HG3	1:A:50:ARG:N	1.82	0.90
1:A:77:ALA:H	1:A:78:THR:HA	1.35	0.90
1:A:265:GLU:CB	1:A:266:HIS:HB2	2.03	0.88
1:A:45:ASP:HB3	1:A:46:GLU:C	2.01	0.85
1:A:160:ILE:HB	1:A:161:ALA:CA	2.00	0.85
1:A:46:GLU:CA	1:A:49:ARG:HD2	2.07	0.84
1:A:106:GLY:O	1:A:109:HIS:HB2	1.79	0.83
1:A:89:MET:O	1:A:89:MET:HG3	1.78	0.83
1:A:334:LEU:HD11	1:A:351:ALA:HB1	1.62	0.81
1:A:77:ALA:H	1:A:78:THR:CA	1.94	0.78
1:A:265:GLU:HB2	1:A:266:HIS:CB	2.13	0.78
1:A:346:ARG:HG2	1:A:346:ARG:NH2	1.82	0.77
1:A:83:VAL:HG22	1:A:152:ASP:HB2	1.68	0.76
1:A:97:THR:HG23	1:A:98:ALA:CB	2.12	0.75
1:A:346:ARG:HH21	1:A:346:ARG:CG	1.98	0.75
1:A:20:LEU:O	1:A:24:VAL:HG23	1.87	0.75
1:A:48:LEU:N	1:A:49:ARG:CB	2.32	0.74
1:A:80:PHE:CB	1:A:151:GLU:HB3	2.14	0.73
1:A:209:ASN:OD1	1:A:212:ASN:HB3	1.87	0.73
1:A:13:VAL:HA	1:A:16:GLN:HG2	1.69	0.73
1:A:134:ARG:HH11	1:A:140:ARG:NH2	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TYR:O	1:A:270:ALA:HB3	1.89	0.72
1:A:265:GLU:CB	1:A:266:HIS:CB	2.68	0.72
1:A:97:THR:CG2	1:A:98:ALA:HB3	2.15	0.72
1:A:121:GLU:OE2	1:A:300:LYS:HD2	1.90	0.72
1:A:77:ALA:H	1:A:79:ASP:N	1.88	0.71
1:A:372:SER:O	1:A:376:ARG:HG2	1.90	0.71
1:A:264:SER:CB	1:A:265:GLU:CA	2.67	0.71
1:A:77:ALA:H	1:A:79:ASP:H	1.38	0.71
1:A:374:ILE:O	1:A:376:ARG:N	2.25	0.70
1:A:358:VAL:HG13	1:A:389:LYS:HZ1	1.53	0.69
1:A:74:ALA:N	1:A:80:PHE:CZ	2.59	0.69
1:A:373:GLU:O	1:A:374:ILE:O	2.11	0.69
1:A:125:ASP:OD2	1:A:295:ASP:OD1	2.11	0.69
1:A:195:LEU:CD1	1:A:229:ARG:HD2	2.20	0.69
1:A:48:LEU:H	1:A:49:ARG:HB3	0.66	0.68
1:A:257:ARG:HB3	1:A:257:ARG:CZ	2.24	0.68
1:A:160:ILE:HG22	1:A:161:ALA:C	2.19	0.68
1:A:284:GLY:N	1:A:287:ARG:HB3	2.05	0.67
1:A:73:GLY:O	1:A:80:PHE:HZ	1.78	0.67
1:A:248:THR:O	1:A:251:GLN:HB2	1.94	0.67
1:A:393:VAL:HG13	1:A:394:ILE:H	1.59	0.67
1:A:380:LEU:CD1	1:A:409:GLU:HG2	2.25	0.66
1:A:339:VAL:HG11	1:A:347:ILE:HD13	1.77	0.66
1:A:381:ILE:O	1:A:409:GLU:HB2	1.95	0.66
1:A:246:PRO:HG2	1:A:252:ALA:HB2	1.78	0.66
1:A:250:HIS:CG	1:A:250:HIS:O	2.48	0.66
1:A:20:LEU:HD22	1:A:51:LEU:HB2	1.78	0.65
1:A:205:ALA:HB1	1:A:206:PRO:HD2	1.77	0.65
1:A:339:VAL:HG12	1:A:340:ASN:N	2.10	0.64
1:A:77:ALA:HB3	1:A:221:LYS:HG3	1.79	0.64
1:A:160:ILE:CB	1:A:161:ALA:CA	2.68	0.64
1:A:303:GLU:HB2	1:A:306:LEU:HD23	1.79	0.64
1:A:336:ASP:HB3	1:A:338:ARG:HH11	1.62	0.64
1:A:287:ARG:HB2	1:A:294:ILE:HD11	1.79	0.64
1:A:336:ASP:HB3	1:A:338:ARG:NH1	2.12	0.64
1:A:49:ARG:CG	1:A:50:ARG:N	2.47	0.64
1:A:312:SER:CB	1:A:317:PRO:HA	2.28	0.63
1:A:49:ARG:HG3	1:A:50:ARG:HD2	1.79	0.63
1:A:264:SER:HB3	1:A:265:GLU:HA	1.77	0.63
1:A:269:LEU:CA	1:A:270:ALA:CB	2.74	0.63
1:A:77:ALA:N	1:A:78:THR:CA	2.54	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:O	1:A:59:PRO:HA	2.00	0.62
1:A:187:PHE:HA	1:A:230:ARG:NH1	2.14	0.62
1:A:46:GLU:C	1:A:49:ARG:HD2	2.24	0.61
1:A:134:ARG:HE	1:A:140:ARG:HH21	1.49	0.61
1:A:265:GLU:HB2	1:A:266:HIS:CA	2.31	0.61
1:A:46:GLU:HA	1:A:49:ARG:CD	2.20	0.61
1:A:47:LEU:HA	1:A:49:ARG:HG2	1.82	0.60
1:A:328:GLU:OE1	1:A:388:ARG:NH1	2.34	0.60
1:A:233:MET:HE3	1:A:233:MET:HA	1.84	0.60
1:A:58:HIS:ND1	1:A:58:HIS:N	2.50	0.60
1:A:42:ALA:HA	1:A:43:GLU:C	2.26	0.60
1:A:98:ALA:O	1:A:99:ASP:CG	2.45	0.59
1:A:306:LEU:HA	1:A:309:ARG:HB3	1.85	0.59
1:A:363:VAL:HG21	1:A:395:PRO:HG2	1.85	0.59
1:A:91:SER:OG	1:A:92:LEU:N	2.30	0.58
1:A:134:ARG:HH11	1:A:140:ARG:HH22	1.50	0.58
1:A:57:GLN:HA	1:A:59:PRO:HD3	1.85	0.58
1:A:118:TYR:O	1:A:270:ALA:CB	2.51	0.58
1:A:264:SER:HB3	1:A:265:GLU:CG	2.29	0.58
1:A:102:ALA:O	1:A:106:GLY:N	2.32	0.58
1:A:265:GLU:HB3	1:A:266:HIS:HB2	1.84	0.58
1:A:220:GLN:NE2	1:A:225:VAL:HG11	2.19	0.57
1:A:158:ARG:NH1	1:A:165:GLU:CD	2.63	0.57
1:A:199:LEU:O	1:A:200:VAL:HB	2.04	0.57
1:A:233:MET:O	1:A:262:PRO:HB2	2.05	0.57
1:A:257:ARG:HB3	1:A:257:ARG:NH1	2.20	0.57
1:A:265:GLU:HB2	1:A:266:HIS:C	2.29	0.57
1:A:339:VAL:CG1	1:A:340:ASN:H	2.15	0.57
1:A:41:ASP:HB3	1:A:44:PHE:O	2.04	0.57
1:A:311:GLY:O	1:A:318:ARG:HB2	2.05	0.57
1:A:13:VAL:HG12	1:A:61:LEU:HD11	1.88	0.56
1:A:77:ALA:H	1:A:78:THR:C	2.13	0.56
1:A:76:PHE:HA	1:A:80:PHE:H	1.71	0.56
1:A:101:LEU:O	1:A:103:ALA:N	2.35	0.56
1:A:217:SER:O	1:A:226:THR:HG23	2.07	0.55
1:A:116:ALA:O	1:A:117:HIS:HB2	2.06	0.55
1:A:200:VAL:O	1:A:205:ALA:HA	2.06	0.55
1:A:113:GLY:O	1:A:115:ALA:N	2.39	0.55
1:A:264:SER:HB3	1:A:265:GLU:CA	2.36	0.55
1:A:374:ILE:HG22	1:A:375:LYS:H	1.72	0.55
1:A:76:PHE:HB3	1:A:81:GLU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASP:C	1:A:408:SER:H	2.14	0.55
1:A:204:LYS:N	3:A:628:HOH:O	2.31	0.55
1:A:336:ASP:OD1	1:A:338:ARG:HD2	2.07	0.55
1:A:48:LEU:CA	1:A:49:ARG:HB3	2.32	0.55
1:A:325:TYR:HB3	1:A:326:PRO:CD	2.36	0.55
1:A:265:GLU:HB3	1:A:266:HIS:CD2	2.42	0.54
1:A:13:VAL:HA	1:A:16:GLN:CG	2.38	0.54
1:A:101:LEU:C	1:A:103:ALA:H	2.15	0.54
1:A:265:GLU:HB3	1:A:266:HIS:CG	2.43	0.54
1:A:101:LEU:HD12	1:A:102:ALA:H	1.73	0.54
1:A:165:GLU:HB2	1:A:166:ARG:HE	1.72	0.54
1:A:112:VAL:HG23	1:A:310:LEU:HD13	1.90	0.53
1:A:225:VAL:O	1:A:228:ARG:HG2	2.07	0.53
2:A:616:AMP:H2'	2:A:616:AMP:N3	2.23	0.53
1:A:200:VAL:HG12	1:A:201:GLU:HG2	1.90	0.53
1:A:78:THR:O	1:A:220:GLN:O	2.27	0.53
1:A:96:PHE:HD2	1:A:99:ASP:OD1	1.92	0.53
1:A:158:ARG:HH12	1:A:160:ILE:HD11	1.74	0.53
1:A:85:HIS:CD2	1:A:147:GLY:O	2.62	0.53
1:A:107:ARG:HH11	1:A:110:ALA:HB2	1.74	0.53
1:A:349:PRO:HG3	1:A:374:ILE:HD11	1.89	0.53
1:A:380:LEU:O	1:A:383:ASP:HB2	2.09	0.53
1:A:248:THR:HB	1:A:302:ASP:CG	2.33	0.52
1:A:405:ARG:C	1:A:407:GLY:H	2.18	0.52
1:A:244:PHE:CG	1:A:245:ARG:N	2.77	0.52
1:A:325:TYR:HB3	1:A:326:PRO:HD2	1.91	0.52
1:A:82:PRO:HA	1:A:150:GLY:O	2.10	0.51
1:A:220:GLN:HE21	1:A:225:VAL:HG11	1.75	0.51
1:A:101:LEU:C	1:A:103:ALA:N	2.68	0.51
1:A:139:THR:O	1:A:154:THR:HG21	2.11	0.51
1:A:391:GLY:HA3	1:A:393:VAL:N	2.25	0.51
1:A:83:VAL:CG2	1:A:152:ASP:HB2	2.39	0.51
1:A:403:GLU:CD	1:A:403:GLU:H	2.18	0.51
1:A:197:ALA:HA	1:A:200:VAL:HG23	1.93	0.51
1:A:374:ILE:O	1:A:375:LYS:C	2.54	0.50
1:A:47:LEU:O	1:A:48:LEU:HB2	2.10	0.50
1:A:132:VAL:HG23	1:A:140:ARG:O	2.11	0.50
1:A:333:LYS:HD3	1:A:384:THR:HG23	1.93	0.50
1:A:94:ASN:ND2	1:A:324:LYS:HE2	2.27	0.50
1:A:112:VAL:HG23	1:A:310:LEU:CD1	2.42	0.50
1:A:100:GLU:HA	1:A:101:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ILE:HA	1:A:351:ALA:HA	1.93	0.50
1:A:78:THR:O	1:A:221:LYS:HA	2.12	0.49
1:A:116:ALA:O	1:A:117:HIS:ND1	2.44	0.49
1:A:116:ALA:O	1:A:117:HIS:CB	2.59	0.49
1:A:370:ASN:O	1:A:374:ILE:HG13	2.12	0.49
1:A:11:PRO:HD2	1:A:13:VAL:HG23	1.95	0.49
1:A:45:ASP:HA	1:A:46:GLU:HG2	1.95	0.49
1:A:296:GLY:HA2	1:A:325:TYR:CD2	2.47	0.49
1:A:129:LEU:CD1	1:A:131:LEU:HG	2.44	0.48
1:A:210:PRO:HA	1:A:213:SER:HB3	1.95	0.48
1:A:77:ALA:N	1:A:79:ASP:H	2.07	0.48
1:A:199:LEU:CD1	1:A:200:VAL:H	2.26	0.48
1:A:230:ARG:HE	1:A:231:LEU:H	1.61	0.48
1:A:73:GLY:C	1:A:80:PHE:HZ	2.20	0.48
1:A:125:ASP:HB2	1:A:293:GLU:HG2	1.95	0.48
1:A:45:ASP:CB	1:A:46:GLU:O	2.49	0.48
1:A:136:GLY:O	1:A:166:ARG:HA	2.14	0.48
1:A:97:THR:O	1:A:323:TYR:CZ	2.67	0.47
1:A:250:HIS:H	1:A:251:GLN:HB2	1.79	0.47
1:A:48:LEU:HG	1:A:48:LEU:O	2.13	0.47
1:A:101:LEU:CG	1:A:102:ALA:H	2.27	0.47
1:A:125:ASP:OD1	1:A:211:ARG:HB2	2.14	0.47
1:A:265:GLU:HB3	1:A:266:HIS:CB	2.39	0.47
1:A:96:PHE:HB2	1:A:99:ASP:OD1	2.14	0.47
1:A:217:SER:OG	1:A:229:ARG:NH1	2.48	0.47
1:A:226:THR:HG22	1:A:231:LEU:HD11	1.96	0.47
1:A:339:VAL:HG11	1:A:347:ILE:CD1	2.43	0.47
1:A:101:LEU:CD1	1:A:102:ALA:H	2.28	0.47
1:A:373:GLU:C	1:A:374:ILE:O	2.58	0.47
1:A:380:LEU:HD13	1:A:409:GLU:HG2	1.96	0.46
1:A:312:SER:HB3	1:A:317:PRO:HA	1.98	0.46
1:A:92:LEU:HD13	1:A:298:VAL:HG21	1.97	0.46
1:A:375:LYS:C	1:A:377:LYS:H	2.24	0.46
1:A:385:VAL:HG13	1:A:397:VAL:HG13	1.98	0.46
1:A:132:VAL:HG21	1:A:140:ARG:HD2	1.96	0.46
1:A:186:PHE:CE1	1:A:232:ARG:HB2	2.51	0.46
1:A:342:GLY:HA2	1:A:343:ARG:NH1	2.31	0.46
1:A:393:VAL:HG13	1:A:394:ILE:N	2.27	0.46
1:A:211:ARG:HD2	1:A:211:ARG:O	2.16	0.45
1:A:13:VAL:CA	1:A:16:GLN:HG2	2.45	0.45
1:A:168:THR:HA	1:A:169:PRO:HD3	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TRP:CZ2	1:A:320:ALA:HA	2.52	0.45
1:A:298:VAL:HG11	2:A:616:AMP:C6	2.51	0.45
1:A:257:ARG:HH12	1:A:263:VAL:H	1.65	0.45
1:A:257:ARG:NH1	1:A:263:VAL:H	2.15	0.44
1:A:86:LEU:HD12	1:A:180:GLU:HB2	1.99	0.44
1:A:108:ILE:O	1:A:109:HIS:C	2.61	0.44
1:A:250:HIS:HB3	3:A:618:HOH:O	2.16	0.44
1:A:372:SER:O	1:A:373:GLU:C	2.60	0.44
1:A:101:LEU:HG	1:A:102:ALA:H	1.81	0.44
1:A:230:ARG:HH12	1:A:232:ARG:HG2	1.83	0.44
1:A:10:ALA:HA	1:A:11:PRO:HD3	1.71	0.44
1:A:175:VAL:HA	1:A:176:PRO:HD3	1.93	0.43
1:A:287:ARG:NH1	1:A:325:TYR:HB3	2.33	0.43
1:A:246:PRO:HB3	1:A:251:GLN:HB3	2.00	0.43
1:A:104:TRP:HZ2	1:A:320:ALA:HA	1.83	0.43
1:A:160:ILE:H	1:A:160:ILE:HG12	1.51	0.43
1:A:230:ARG:NE	1:A:231:LEU:H	2.16	0.43
1:A:414:MET:HA	1:A:415:PRO:HD3	1.76	0.43
1:A:265:GLU:CB	1:A:266:HIS:CA	2.95	0.43
1:A:338:ARG:HG2	1:A:352:PHE:CD2	2.54	0.43
1:A:339:VAL:HG21	1:A:414:MET:HG2	2.01	0.43
1:A:131:LEU:HD21	1:A:163:VAL:HG21	2.00	0.43
1:A:36:ALA:N	1:A:37:PRO:HD3	2.34	0.42
1:A:79:ASP:O	1:A:80:PHE:HB3	2.19	0.42
1:A:414:MET:SD	1:A:415:PRO:HD2	2.58	0.42
1:A:100:GLU:H	1:A:100:GLU:HG2	1.59	0.42
1:A:104:TRP:CD1	1:A:321:ILE:HG23	2.54	0.42
1:A:347:ILE:H	1:A:347:ILE:HG13	1.70	0.42
1:A:287:ARG:HB2	1:A:294:ILE:CD1	2.47	0.42
1:A:386:VAL:HG23	1:A:398:LEU:HB2	2.02	0.42
1:A:257:ARG:HD2	1:A:263:VAL:HG22	2.02	0.42
1:A:73:GLY:HA3	1:A:74:ALA:HA	1.76	0.42
1:A:85:HIS:CE1	1:A:89:MET:HE3	2.54	0.42
1:A:230:ARG:CZ	1:A:230:ARG:HB2	2.49	0.42
1:A:124:ILE:H	1:A:124:ILE:HG12	1.39	0.42
1:A:217:SER:O	1:A:226:THR:CG2	2.68	0.42
1:A:391:GLY:HA3	1:A:393:VAL:H	1.83	0.42
1:A:164:PRO:HB2	1:A:166:ARG:O	2.19	0.42
1:A:46:GLU:O	1:A:47:LEU:C	2.63	0.42
1:A:104:TRP:CD2	1:A:321:ILE:HG13	2.55	0.42
1:A:163:VAL:HA	1:A:164:PRO:HD3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:CZ	1:A:182:ARG:HB3	2.50	0.42
1:A:250:HIS:HD2	1:A:253:TYR:HB2	1.85	0.42
1:A:272:ASP:OD2	1:A:273:LEU:N	2.52	0.41
1:A:280:ILE:HG23	1:A:323:TYR:CE2	2.54	0.41
1:A:286:HIS:O	1:A:289:GLU:HG2	2.20	0.41
1:A:293:GLU:HG3	1:A:328:GLU:OE2	2.19	0.41
1:A:406:ASP:O	1:A:408:SER:N	2.53	0.41
1:A:79:ASP:C	1:A:80:PHE:CD2	2.98	0.41
1:A:248:THR:HB	1:A:302:ASP:OD2	2.20	0.41
1:A:371:ALA:HA	1:A:374:ILE:HD12	2.03	0.41
1:A:89:MET:HB3	1:A:147:GLY:O	2.20	0.41
1:A:406:ASP:C	1:A:408:SER:N	2.78	0.41
1:A:90:LEU:HD13	1:A:313:THR:O	2.21	0.40
1:A:226:THR:CG2	1:A:231:LEU:HD11	2.51	0.40
1:A:134:ARG:HD2	1:A:139:THR:HG21	2.03	0.40
1:A:204:LYS:HB3	1:A:205:ALA:H	1.63	0.40
1:A:233:MET:HA	1:A:233:MET:CE	2.51	0.40
1:A:248:THR:OG1	1:A:251:GLN:HG2	2.10	0.40
1:A:35:ASP:OD1	1:A:35:ASP:N	2.54	0.40
1:A:312:SER:HA	1:A:318:ARG:H	1.86	0.40
1:A:363:VAL:HG22	1:A:365:GLN:H	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:CZ	1:A:171:ASP:OD1[4_455]	2.15	0.05

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	406/615 (66%)	304 (75%)	57 (14%)	45 (11%)	0 5

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	46	GLU
1	A	47	LEU
1	A	48	LEU
1	A	49	ARG
1	A	88	ARG
1	A	99	ASP
1	A	114	ASP
1	A	115	ALA
1	A	117	HIS
1	A	160	ILE
1	A	171	ASP
1	A	172	ASP
1	A	245	ARG
1	A	270	ALA
1	A	291	ASP
1	A	374	ILE
1	A	375	LYS
1	A	393	VAL
1	A	414	MET
1	A	11	PRO
1	A	57	GLN
1	A	69	GLN
1	A	73	GLY
1	A	101	LEU
1	A	269	LEU
1	A	413	ILE
1	A	42	ALA
1	A	109	HIS
1	A	204	LYS
1	A	208	ALA
1	A	244	PHE
1	A	246	PRO
1	A	345	GLY
1	A	376	ARG
1	A	407	GLY
1	A	80	PHE
1	A	83	VAL

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Mol	Chain	Res	Type
1	A	98	ALA
1	A	159	THR
1	A	231	LEU
1	A	344	THR
1	A	102	ALA
1	A	110	ALA
1	A	71	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	328/492 (67%)	246 (75%)	82 (25%)	0 4

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	16	GLN
1	A	20	LEU
1	A	35	ASP
1	A	50	ARG
1	A	58	HIS
1	A	62	ARG
1	A	68	THR
1	A	78	THR
1	A	83	VAL
1	A	84	ASP
1	A	93	ASP
1	A	96	PHE
1	A	97	THR
1	A	108	ILE
1	A	109	HIS
1	A	111	GLU
1	A	112	VAL
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	121	GLU
1	A	124	ILE
1	A	125	ASP
1	A	132	VAL
1	A	137	ARG
1	A	140	ARG
1	A	148	ARG
1	A	149	THR
1	A	155	LEU
1	A	158	ARG
1	A	160	ILE
1	A	165	GLU
1	A	166	ARG
1	A	178	VAL
1	A	189	LEU
1	A	192	PHE
1	A	199	LEU
1	A	212	ASN
1	A	226	THR
1	A	229	ARG
1	A	230	ARG
1	A	233	MET
1	A	238	LEU
1	A	249	LEU
1	A	251	GLN
1	A	254	LEU
1	A	256	LEU
1	A	257	ARG
1	A	263	VAL
1	A	264	SER
1	A	266	HIS
1	A	268	THR
1	A	271	THR
1	A	272	ASP
1	A	279	ARG
1	A	285	GLU
1	A	287	ARG
1	A	290	VAL
1	A	301	VAL
1	A	306	LEU
1	A	310	LEU
1	A	324	LYS

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Mol	Chain	Res	Type
1	A	338	ARG
1	A	341	VAL
1	A	346	ARG
1	A	347	ILE
1	A	354	THR
1	A	356	VAL
1	A	357	LYS
1	A	358	VAL
1	A	365	GLN
1	A	368	LEU
1	A	374	ILE
1	A	380	LEU
1	A	385	VAL
1	A	394	ILE
1	A	398	LEU
1	A	401	VAL
1	A	403	GLU
1	A	405	ARG
1	A	409	GLU
1	A	411	GLU
1	A	413	ILE

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

Mol	Chain	Res	Type
1	A	8	GLN
1	A	57	GLN
1	A	109	HIS
1	A	156	ASN
1	A	212	ASN
1	A	220	GLN
1	A	236	HIS
1	A	240	HIS
1	A	266	HIS
1	A	286	HIS
1	A	340	ASN
1	A	365	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	AMP	A	616	1	21,24,25	1.92	7 (33%)	30,35,38	2.29	12 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	A	616	1	-	3/7/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	616	AMP	C5-N7	-4.33	1.31	1.39
2	A	616	AMP	C8-N9	-3.16	1.32	1.37
2	A	616	AMP	C4-N9	-2.98	1.31	1.37
2	A	616	AMP	C5-C4	2.75	1.44	1.39
2	A	616	AMP	P-O5'	-2.44	1.56	1.62
2	A	616	AMP	O4'-C4'	-2.29	1.39	1.45
2	A	616	AMP	C3'-C4'	-2.25	1.47	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	616	AMP	C5-C4-N3	-6.15	118.24	126.72
2	A	616	AMP	N3-C4-N9	5.03	135.71	127.17
2	A	616	AMP	C2-N3-C4	3.75	120.98	111.83
2	A	616	AMP	N3-C2-N1	-3.47	123.33	128.58
2	A	616	AMP	C4-C5-N7	-3.07	107.07	110.58
2	A	616	AMP	O3'-C3'-C4'	-2.67	103.41	111.08
2	A	616	AMP	C4-N9-C8	2.64	108.51	105.74
2	A	616	AMP	C5-N7-C8	2.60	107.53	103.45
2	A	616	AMP	O2'-C2'-C3'	-2.21	104.75	111.82
2	A	616	AMP	N9-C8-N7	-2.18	110.84	113.94
2	A	616	AMP	O4'-C4'-C3'	-2.13	100.92	105.15
2	A	616	AMP	C2-N1-C6	2.04	122.08	118.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

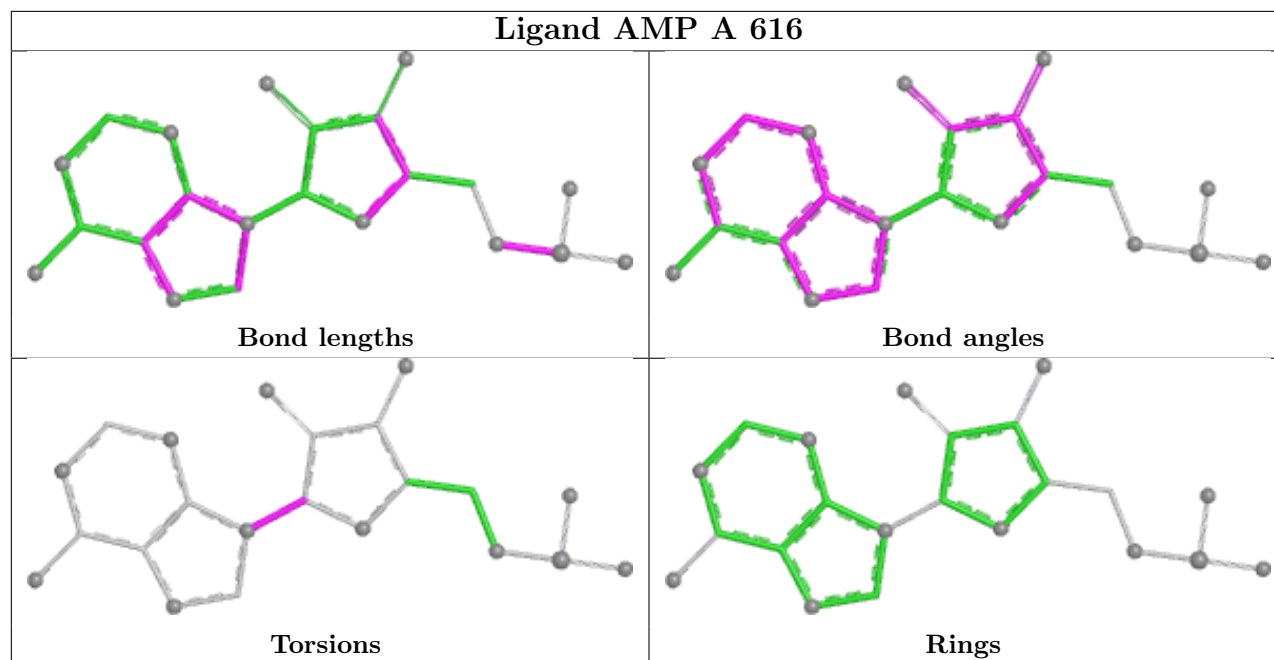
Mol	Chain	Res	Type	Atoms
2	A	616	AMP	C2'-C1'-N9-C4
2	A	616	AMP	C2'-C1'-N9-C8
2	A	616	AMP	O4'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	616	AMP	2	0

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



5.7 Other polymers [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	408/615 (66%)	0.76	34 (8%) 17 11	23, 52, 74, 78	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	ALA	4.2
1	A	79	ASP	4.0
1	A	203	GLY	3.7
1	A	109	HIS	3.4
1	A	265	GLU	3.3
1	A	47	LEU	3.3
1	A	278	GLU	3.2
1	A	390	ALA	3.2
1	A	347	ILE	3.2
1	A	341	VAL	3.0
1	A	111	GLU	2.9
1	A	172	ASP	2.7
1	A	74	ALA	2.6
1	A	198	SER	2.6
1	A	345	GLY	2.5
1	A	71	VAL	2.5
1	A	202	GLU	2.5
1	A	400	PRO	2.5
1	A	60	GLU	2.5
1	A	67	PRO	2.4
1	A	342	GLY	2.4
1	A	350	PHE	2.3
1	A	211	ARG	2.3
1	A	98	ALA	2.3
1	A	219	ARG	2.3
1	A	218	LEU	2.2
1	A	59	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	165	GLU	2.2
1	A	230	ARG	2.1
1	A	250	HIS	2.1
1	A	389	LYS	2.1
1	A	410	ARG	2.1
1	A	12	GLU	2.0
1	A	290	VAL	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](#)

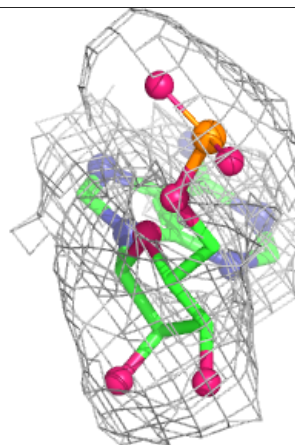
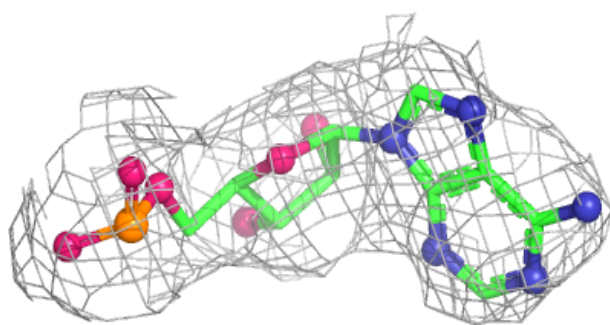
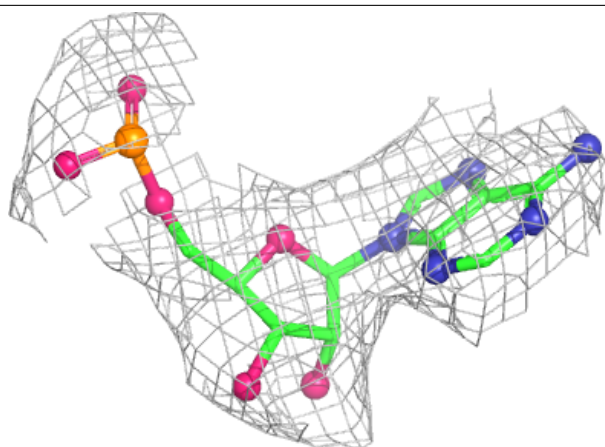
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	AMP	A	616	22/23	0.93	0.10	45,49,55,56	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 AMP A 616:

$2mF_o-DF_c$ (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.