



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:27 AM UTC

PDB ID : 2J9D / pdb_00002j9d
Title : Structure of GlnK1 with bound effectors indicates regulatory mechanism for ammonia uptake
Authors : Yildiz, O.; Kalthoff, C.; Raunser, S.; Kuehlbrandt, W.
Deposited on : 2006-11-07
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

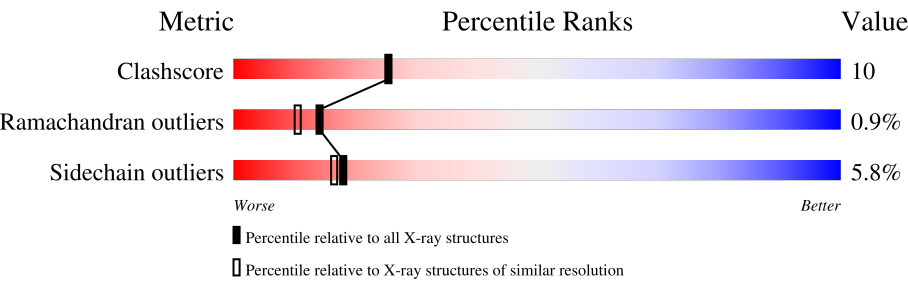
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	72% 13% • 14%
1	B	119	72% 10% • • 13%
1	C	119	74% 22% • •
1	D	119	68% 18% • 13%
1	F	119	82% 10% • 5%
1	G	119	74% 12% • 13%
1	H	119	70% 14% • 15%
1	I	119	76% 18% • •

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Mol	Chain	Length	Quality of chain
1	J	119	
1	K	119	
1	L	119	
2	E	119	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	1116	-	-	X	-
3	ACT	A	1117	-	-	X	-
3	ACT	E	1116	-	-	X	-
3	ACT	H	1113	-	-	X	-
3	ACT	J	1116	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10840 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 HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	4	0
			779	491	135	150	3			
1	B	103	Total	C	N	O	S	0	0	0
			788	498	136	151	3			
1	C	116	Total	C	N	O	S	0	0	0
			897	566	158	170	3			
1	D	103	Total	C	N	O	S	0	0	0
			789	497	138	151	3			
1	F	113	Total	C	N	O	S	0	0	0
			880	557	155	165	3			
1	G	103	Total	C	N	O	S	0	0	0
			784	496	136	149	3			
1	H	101	Total	C	N	O	S	0	0	0
			772	488	134	147	3			
1	I	116	Total	C	N	O	S	0	0	0
			874	550	153	168	3			
1	J	115	Total	C	N	O	S	0	0	0
			870	546	158	163	3			
1	K	102	Total	C	N	O	S	0	0	0
			779	491	135	150	3			
1	L	115	Total	C	N	O	S	0	0	0
			887	560	158	166	3			

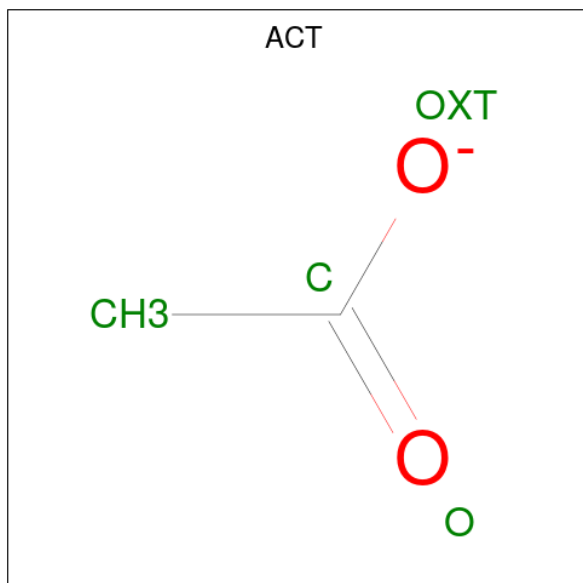
- Molecule 2 is a protein called HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	116	Total	C	N	O	S	0	0	0
			895	563	156	173	3			

There is a discrepancy between the modelled and reference sequences:

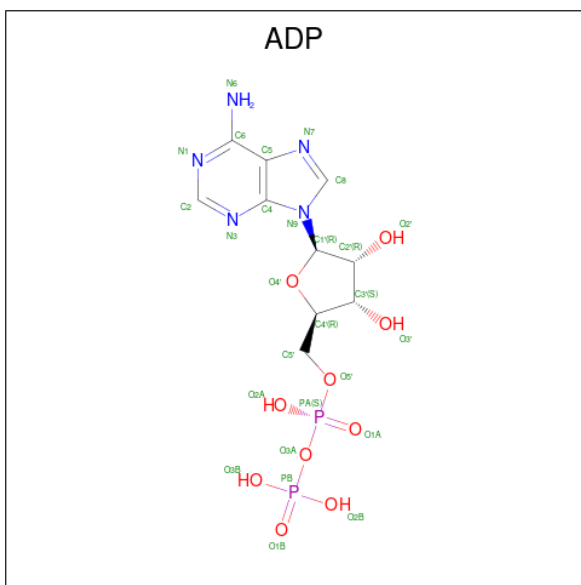
Chain	Residue	Modelled	Actual	Comment	Reference
E	113	GLU	LEU	conflict	UNP Q60381

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



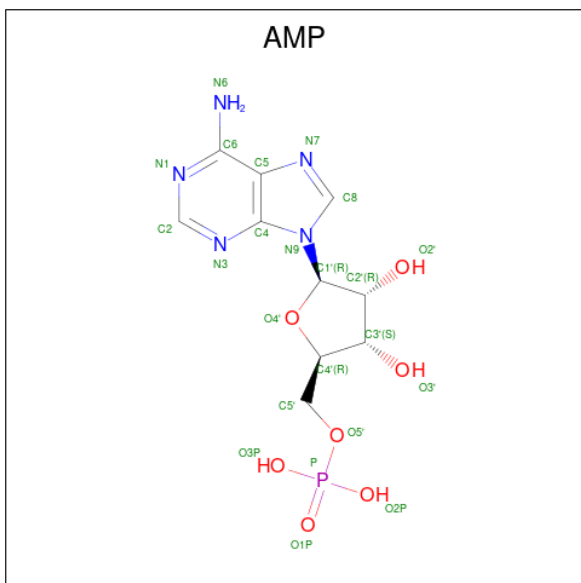
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	L	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	57	Total	O	0	0
			57	57		
7	B	78	Total	O	0	0
			78	78		
7	C	60	Total	O	0	0
			60	60		
7	D	64	Total	O	0	0
			64	64		
7	E	75	Total	O	0	0
			75	75		
7	F	64	Total	O	0	0
			64	64		
7	G	41	Total	O	0	0
			41	41		
7	H	51	Total	O	0	0
			51	51		
7	I	42	Total	O	0	0
			42	42		
7	J	44	Total	O	0	0
			44	44		
7	K	45	Total	O	0	0
			45	45		
7	L	73	Total	O	0	0
			73	73		

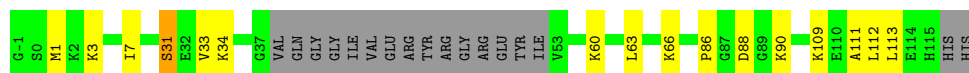
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

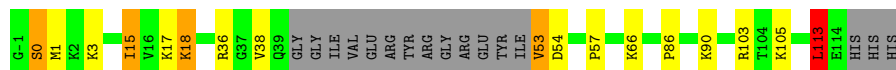
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain A: 



• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain B: 



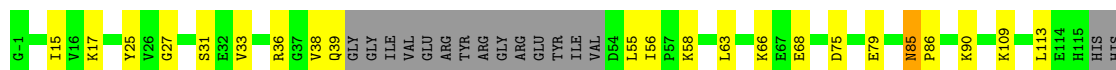
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain C: 



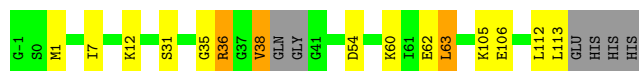
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain D: 



• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain F: 



• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain G: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.60Å 107.03Å 134.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 2.10	Depositor
% Data completeness (in resolution range)	100.0 (19.78-2.10)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10840	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CL, ACT, 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	0.75	0/783	0.86	0/1049
1	B	0.76	0/792	0.88	0/1062
1	C	0.72	0/904	0.87	1/1212 (0.1%)
1	D	0.74	0/794	0.93	2/1064 (0.2%)
1	F	0.72	0/886	0.83	0/1187
1	G	0.72	0/788	0.92	0/1057
1	H	0.75	0/776	0.87	0/1040
1	I	0.72	0/880	0.81	0/1182
1	J	0.72	0/876	0.85	0/1175
1	K	0.79	0/783	0.89	1/1049 (0.1%)
1	L	0.77	1/894 (0.1%)	0.88	0/1199
2	E	0.78	0/902	0.87	0/1210
All	All	0.75	1/10058 (0.0%)	0.87	4/13486 (0.0%)

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	D	0	1
1	K	0	1
1	L	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	94	ILE	CA-CB	6.12	1.59	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	34	LYS	O-C-N	-5.71	116.30	123.27
1	C	39	GLN	N-CA-C	5.29	117.59	109.07
1	D	85	ASN	CA-C-N	5.25	126.40	119.84
1	D	85	ASN	C-N-CA	5.25	126.40	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	85	ASN	Peptide
1	K	34	LYS	Peptide
1	L	51	TYR	Peptide

5.2 Too-close contacts [i](#)

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	779	0	814	14	0
1	B	788	0	843	14	0
1	C	897	0	952	31	0
1	D	789	0	834	16	0
1	F	880	0	941	15	0
1	G	784	0	839	17	0
1	H	772	0	828	17	0
1	I	874	0	910	24	0
1	J	870	0	913	25	0
1	K	779	0	827	27	0
1	L	887	0	942	25	0
2	E	895	0	936	21	0
3	A	8	0	6	9	0
3	E	4	0	3	7	0
3	H	4	0	3	4	0
3	J	4	0	3	3	0
4	B	27	0	12	1	0
4	I	27	0	12	0	0
4	J	27	0	12	1	0
4	L	27	0	12	0	0
5	E	23	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1	0	0	1	0
7	A	57	0	0	2	0
7	B	78	0	0	1	0
7	C	60	0	0	3	0
7	D	64	0	0	0	0
7	E	75	0	0	0	0
7	F	64	0	0	2	0
7	G	41	0	0	0	0
7	H	51	0	0	0	0
7	I	42	0	0	0	0
7	J	44	0	0	1	0
7	K	45	0	0	0	0
7	L	73	0	0	1	0
All	All	10840	0	10654	199	0

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 10.

All (199) 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:H:3:LYS:HZ1	3:H:1113:ACT:H1	1.21	1.05
1:C:27:GLY:O	1:C:63:LEU:CD1	2.12	0.97
1:L:63:LEU:HD23	1:L:65:VAL:HG13	1.50	0.94
1:D:27:GLY:O	1:D:63:LEU:CD1	2.17	0.93
1:C:28:MET:HE3	1:C:61:ILE:HG23	1.49	0.92
1:L:42:ILE:HA	1:L:43:VAL:CB	2.00	0.89
1:C:27:GLY:O	1:C:63:LEU:HD12	1.73	0.88
1:J:27:GLY:O	1:J:63:LEU:CD1	2.21	0.88
1:F:1:MET:HE1	1:F:112:LEU:HD21	1.57	0.87
1:K:26:VAL:O	1:L:36:ARG:HD2	1.74	0.86
1:J:42:ILE:HA	1:J:43:VAL:CB	2.05	0.86
1:J:27:GLY:O	1:J:63:LEU:HD13	1.76	0.85
2:E:5:GLU:OE1	3:E:1116:ACT:H1	1.76	0.85
1:L:1:MET:CE	1:L:112:LEU:HD12	2.08	0.84
1:I:27:GLY:O	1:I:63:LEU:HD13	1.78	0.82
1:I:41:GLY:HA2	1:I:42:ILE:HG22	1.58	0.82
1:C:63:LEU:HD11	7:C:2010:HOH:O	1.80	0.81
1:H:3:LYS:NZ	3:H:1113:ACT:H1	1.94	0.81
1:K:35:GLY:HA2	1:K:56:ILE:O	1.81	0.80
1:F:1:MET:CE	1:F:112:LEU:HD21	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:LEU:HD21	1:L:65:VAL:HG11	1.63	0.78
1:L:63:LEU:CD2	1:L:65:VAL:CG1	2.62	0.78
1:G:36:ARG:HD2	1:I:27:GLY:HA2	1.65	0.77
1:B:113:LEU:O	1:C:38:VAL:HG21	1.85	0.77
1:L:63:LEU:CD2	1:L:65:VAL:HG13	2.15	0.77
1:K:96:VAL:HG22	1:L:94:ILE:CD1	2.16	0.75
1:G:15:ILE:HD11	1:J:46:TYR:CB	2.17	0.75
1:C:1:MET:HE1	1:C:109:LYS:HZ2	1.52	0.74
3:J:1116:ACT:H1	1:K:5:GLU:OE1	1.88	0.74
1:J:42:ILE:CA	1:J:43:VAL:CB	2.65	0.73
1:L:63:LEU:HD21	1:L:65:VAL:CG1	2.18	0.73
1:C:53:VAL:HG22	2:E:52:ILE:CG2	2.17	0.73
1:G:15:ILE:HD11	1:J:46:TYR:HB2	1.69	0.73
1:K:114:GLU:C	1:L:38:VAL:HG11	2.14	0.73
1:H:27:GLY:O	1:H:63:LEU:HD12	1.90	0.71
1:G:36:ARG:HD3	1:G:36:ARG:H	1.55	0.71
1:I:55:LEU:O	1:I:56:ILE:HD12	1.91	0.71
1:I:42:ILE:O	1:I:42:ILE:HG23	1.90	0.70
1:J:28:MET:HE2	1:J:61:ILE:CG2	2.22	0.70
1:L:1:MET:HE1	1:L:112:LEU:HD12	1.74	0.70
1:I:41:GLY:CA	1:I:42:ILE:HG22	2.21	0.69
1:G:33:VAL:HG12	1:I:31:SER:HB3	1.74	0.69
1:F:1:MET:HE1	1:F:112:LEU:CD2	2.23	0.69
1:D:27:GLY:O	1:D:63:LEU:HD13	1.92	0.68
1:L:63:LEU:HD23	1:L:65:VAL:CG1	2.23	0.67
1:K:1:MET:HE1	1:K:112:LEU:HD12	1.75	0.67
1:C:28:MET:HE3	1:C:61:ILE:CG2	2.24	0.66
1:J:28:MET:HE2	1:J:61:ILE:HG21	1.77	0.66
1:I:27:GLY:O	1:I:63:LEU:CD1	2.44	0.66
1:J:1:MET:HE2	1:J:66:LYS:HA	1.79	0.65
1:C:1:MET:HE1	1:C:109:LYS:NZ	2.12	0.64
1:G:36:ARG:HH11	1:G:36:ARG:HG2	1.63	0.64
3:A:1117:ACT:H2	1:C:103:ARG:HB2	1.80	0.64
1:F:1:MET:HE2	1:F:112:LEU:HD11	1.80	0.64
2:E:3:LYS:NZ	3:E:1116:ACT:H2	2.14	0.62
3:J:1116:ACT:H2	1:K:3:LYS:NZ	2.15	0.62
1:J:28:MET:CE	1:J:61:ILE:HG21	2.30	0.61
1:K:26:VAL:O	1:L:36:ARG:CD	2.47	0.61
1:H:5:GLU:OE2	3:H:1113:ACT:H3	1.99	0.61
1:I:110:GLU:HA	1:I:113:LEU:HD22	1.81	0.61
1:H:28:MET:HE3	1:I:36:ARG:NH1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:46:TYR:CZ	1:K:18:LYS:HD3	2.36	0.61
1:L:42:ILE:CA	1:L:43:VAL:CB	2.78	0.61
1:D:38:VAL:CB	1:D:39:GLN:C	2.74	0.60
1:B:54:ASP:O	7:B:2037:HOH:O	2.16	0.60
1:B:103:ARG:HB3	1:C:88:ASP:OD2	2.01	0.60
1:C:-1:GLY:H3	1:C:109:LYS:HE2	1.66	0.60
1:A:3:LYS:HE3	3:A:1116:ACT:H3	1.84	0.59
1:D:66:LYS:NZ	1:D:68:GLU:OE1	2.36	0.59
1:I:46:TYR:CE1	1:K:18:LYS:HD3	2.37	0.59
1:I:101:ARG:NH2	1:I:113:LEU:O	2.35	0.59
1:I:32:GLU:OE1	1:K:34:LYS:NZ	2.34	0.59
1:G:26:VAL:HG21	1:H:38:VAL:H	1.68	0.58
1:K:1:MET:CE	1:K:112:LEU:HD12	2.32	0.58
1:C:1:MET:CE	1:C:109:LYS:NZ	2.65	0.58
1:L:63:LEU:CD2	1:L:65:VAL:HG11	2.29	0.58
3:J:1116:ACT:H2	1:K:3:LYS:HZ1	1.69	0.58
1:C:52:ILE:HD11	2:E:49:ARG:HG2	1.85	0.57
1:G:36:ARG:H	1:G:36:ARG:CD	2.14	0.57
1:F:62:GLU:OE2	7:F:2037:HOH:O	2.18	0.56
1:D:25:TYR:HB3	1:D:63:LEU:HD21	1.87	0.56
1:H:3:LYS:NZ	3:H:1113:ACT:CH3	2.66	0.56
2:E:3:LYS:HZ1	3:E:1116:ACT:CH3	2.19	0.56
1:C:28:MET:HE2	1:C:30:VAL:CG2	2.36	0.56
1:D:66:LYS:NZ	1:D:68:GLU:CD	2.64	0.55
1:A:3:LYS:NZ	3:A:1116:ACT:H2	2.22	0.55
1:C:1:MET:CE	1:C:109:LYS:HZ2	2.17	0.55
1:L:1:MET:HE2	1:L:112:LEU:HD12	1.88	0.55
1:D:33:VAL:HG12	1:F:31:SER:HB3	1.90	0.54
1:C:53:VAL:HG22	2:E:52:ILE:HG21	1.89	0.54
1:G:15:ILE:HD11	1:J:46:TYR:HB3	1.87	0.53
1:A:3:LYS:HE3	3:A:1116:ACT:CH3	2.39	0.53
1:C:-1:GLY:N	1:C:109:LYS:HE2	2.24	0.52
1:K:109:LYS:O	1:K:113:LEU:HD23	2.08	0.52
1:B:1:MET:HE1	1:B:66:LYS:HG2	1.91	0.52
1:J:60:LYS:NZ	6:J:1114:CL:CL	2.78	0.52
1:I:56:ILE:HD11	1:K:11:GLU:HG2	1.92	0.52
1:B:105:LYS:NZ	1:C:75:ASP:OD1	2.43	0.52
1:C:80:ASN:ND2	7:C:2044:HOH:O	2.42	0.52
1:I:46:TYR:CE2	1:K:18:LYS:HG2	2.44	0.52
1:H:52:ILE:HD12	1:H:52:ILE:O	2.10	0.52
1:F:36:ARG:HD3	1:F:54:ASP:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:ARG:HB2	1:I:55:LEU:HD23	1.92	0.52
1:B:38:VAL:HG23	1:B:86:PRO:HB2	1.91	0.52
1:G:101:ARG:NH2	1:H:90:LYS:NZ	2.57	0.52
1:I:25:TYR:HB3	1:I:63:LEU:HD21	1.92	0.51
1:I:41:GLY:HA3	1:I:42:ILE:C	2.36	0.51
1:D:36:ARG:HG2	1:D:55:LEU:HD23	1.92	0.51
1:J:25:TYR:HB3	1:J:63:LEU:HD21	1.93	0.51
2:E:3:LYS:NZ	3:E:1116:ACT:CH3	2.73	0.51
2:E:3:LYS:HZ1	3:E:1116:ACT:H2	1.74	0.50
1:J:1:MET:CE	1:J:66:LYS:HA	2.41	0.50
1:J:56:ILE:HD11	1:J:58:LYS:HE2	1.93	0.50
1:D:66:LYS:HZ2	1:D:68:GLU:CD	2.19	0.50
2:E:52:ILE:O	2:E:52:ILE:HG23	2.11	0.50
1:K:96:VAL:HG22	1:L:94:ILE:HD11	1.91	0.50
2:E:5:GLU:OE1	3:E:1116:ACT:CH3	2.56	0.49
1:A:33:VAL:HG12	1:C:31:SER:HB3	1.94	0.49
1:B:18:LYS:HE2	2:E:46:TYR:CE1	2.47	0.49
1:B:0:SER:O	1:B:1:MET:HE2	2.13	0.49
1:D:75:ASP:OD1	1:F:105:LYS:NZ	2.45	0.48
1:G:38:VAL:HG23	1:G:86:PRO:HB2	1.95	0.48
1:L:15:ILE:HD12	7:L:2018:HOH:O	2.13	0.48
1:C:105:LYS:CE	7:C:2056:HOH:O	2.61	0.48
1:C:53:VAL:HG22	2:E:52:ILE:HG22	1.92	0.48
1:K:34:LYS:HB3	1:K:55:LEU:HB3	1.95	0.48
1:H:26:VAL:O	1:I:36:ARG:HD2	2.14	0.48
1:J:17:LYS:NZ	1:K:54:ASP:OD1	2.42	0.47
1:A:111:ALA:O	1:B:90:LYS:HE3	2.14	0.47
4:B:1115:ADP:H5'1	1:C:89:GLY:HA2	1.95	0.47
1:H:36:ARG:HB2	1:H:55:LEU:HD23	1.97	0.47
1:K:55:LEU:HD22	1:K:55:LEU:N	2.28	0.47
1:A:90:LYS:HE3	1:C:111:ALA:O	2.15	0.46
1:A:86:PRO:HA	3:A:1117:ACT:H3	1.97	0.46
1:J:103:ARG:NH1	1:K:84:GLY:O	2.49	0.46
1:L:52:ILE:N	1:L:52:ILE:HD12	2.31	0.46
1:C:14:GLU:O	1:C:18:LYS:HD2	2.16	0.45
4:J:1115:ADP:H8	4:J:1115:ADP:H5'1	1.80	0.45
1:K:96:VAL:HG22	1:L:94:ILE:HD13	1.97	0.45
1:A:7:ILE:HD13	1:A:60:LYS:HG3	1.99	0.45
1:H:26:VAL:O	1:I:36:ARG:CD	2.65	0.45
1:L:42:ILE:HD12	1:L:42:ILE:C	2.42	0.45
1:B:38:VAL:CG2	1:B:86:PRO:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:TYR:CD2	1:D:15:ILE:HD11	2.52	0.44
1:A:66:LYS:HD3	1:A:109:LYS:HE3	1.98	0.44
1:D:17:LYS:HE2	2:E:42:ILE:HG23	1.98	0.44
1:K:35:GLY:CA	1:K:56:ILE:O	2.61	0.44
1:B:3:LYS:HE3	1:C:94:ILE:HD11	1.98	0.44
1:C:52:ILE:HD11	2:E:49:ARG:CG	2.48	0.44
2:E:3:LYS:HZ2	3:E:1116:ACT:H2	1.82	0.44
1:I:63:LEU:HG	1:I:65:VAL:HG13	2.00	0.44
1:A:88:ASP:H	3:A:1117:ACT:H1	1.82	0.44
1:I:42:ILE:O	1:I:42:ILE:CG2	2.61	0.44
1:J:28:MET:CE	1:J:61:ILE:CG2	2.91	0.44
1:B:57:PRO:HD2	2:E:10:PRO:HB2	1.99	0.44
2:E:17:LYS:NZ	1:F:54:ASP:OD2	2.41	0.44
1:J:42:ILE:CB	1:J:43:VAL:CB	2.95	0.44
1:F:12:LYS:NZ	7:F:2014:HOH:O	2.42	0.43
1:A:34:LYS:NZ	7:A:2023:HOH:O	2.51	0.43
1:J:31:SER:HB3	1:K:33:VAL:HG12	2.01	0.43
1:I:56:ILE:HD11	1:K:11:GLU:CG	2.48	0.43
1:A:1:MET:SD	1:A:112:LEU:HD11	2.59	0.43
1:B:53:VAL:HG23	2:E:14:GLU:OE1	2.19	0.43
2:E:52:ILE:CG2	2:E:52:ILE:O	2.67	0.43
1:G:38:VAL:CG2	1:G:86:PRO:HB2	2.49	0.43
1:K:112:LEU:O	1:K:114:GLU:N	2.51	0.43
1:D:27:GLY:O	1:D:63:LEU:HD11	2.14	0.42
1:J:63:LEU:HG	1:J:65:VAL:HG13	2.01	0.42
1:F:7:ILE:HD13	1:F:60:LYS:HG3	2.02	0.42
2:E:66:LYS:HD3	2:E:109:LYS:HE3	2.02	0.42
1:G:98:ARG:HB3	1:H:93:VAL:HB	2.01	0.42
1:G:101:ARG:NH2	1:H:90:LYS:HZ1	2.17	0.42
1:C:25:TYR:HB3	1:C:63:LEU:HD21	2.01	0.42
1:D:27:GLY:O	1:D:63:LEU:HD12	2.12	0.42
2:E:40:GLY:H	2:E:53:VAL:HG11	1.84	0.42
1:J:108:GLY:O	1:J:111:ALA:HB3	2.20	0.42
1:H:56:ILE:HD13	1:H:56:ILE:N	2.35	0.42
1:L:52:ILE:HD12	1:L:52:ILE:H	1.85	0.42
5:E:1115:AMP:O3P	1:F:38:VAL:CG1	2.67	0.41
1:L:52:ILE:CD1	1:L:52:ILE:O	2.69	0.41
1:F:63:LEU:N	1:F:63:LEU:HD23	2.35	0.41
1:L:13:LEU:O	1:L:17:LYS:HB2	2.20	0.41
1:B:15:ILE:HD12	1:B:15:ILE:O	2.21	0.41
1:D:56:ILE:HD11	1:D:58:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:VAL:HA	1:D:39:GLN:CB	2.51	0.41
1:C:44:GLU:CD	1:C:45:ARG:H	2.29	0.41
5:E:1115:AMP:O3P	1:F:38:VAL:HG12	2.20	0.41
1:A:3:LYS:HZ1	3:A:1116:ACT:H2	1.86	0.41
1:J:1:MET:HE2	1:J:66:LYS:CA	2.50	0.41
1:G:7:ILE:O	1:G:89:GLY:HA3	2.20	0.41
1:G:26:VAL:HG23	1:H:36:ARG:HD3	2.03	0.41
1:J:34:LYS:NZ	7:J:2015:HOH:O	2.54	0.41
1:K:103:ARG:HB3	1:L:88:ASP:OD2	2.21	0.40
1:A:31[A]:SER:OG	7:A:2021:HOH:O	2.21	0.40
5:E:1115:AMP:O3'	1:F:35:GLY:HA3	2.22	0.40
1:J:7:ILE:CD1	1:J:60:LYS:HG3	2.51	0.40
1:G:105:LYS:NZ	1:H:75:ASP:OD1	2.47	0.40

There are no symmetry-related clashes.

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	98/119 (82%)	98 (100%)	0	0	100	100
1	B	99/119 (83%)	98 (99%)	0	1 (1%)	12	9
1	C	114/119 (96%)	113 (99%)	1 (1%)	0	100	100
1	D	99/119 (83%)	96 (97%)	2 (2%)	1 (1%)	12	9
1	F	109/119 (92%)	104 (95%)	5 (5%)	0	100	100
1	G	99/119 (83%)	98 (99%)	1 (1%)	0	100	100
1	H	97/119 (82%)	96 (99%)	0	1 (1%)	12	9
1	I	114/119 (96%)	109 (96%)	4 (4%)	1 (1%)	14	10
1	J	113/119 (95%)	109 (96%)	2 (2%)	2 (2%)	6	3
1	K	98/119 (82%)	96 (98%)	1 (1%)	1 (1%)	12	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	113/119 (95%)	106 (94%)	3 (3%)	4 (4%)	3	1
2	E	114/119 (96%)	111 (97%)	2 (2%)	1 (1%)	14	10
All	All	1267/1428 (89%)	1234 (97%)	21 (2%)	12 (1%)	14	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	52	ILE
1	J	43	VAL
1	H	37	GLY
1	L	43	VAL
1	L	52	ILE
1	D	86	PRO
1	K	113	LEU
1	L	42	ILE
1	L	50	GLU
1	B	113	LEU
1	J	39	GLN
2	E	42	ILE

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	86/102 (84%)	83 (96%)	3 (4%)	32	35
1	B	88/102 (86%)	81 (92%)	7 (8%)	11	8
1	C	98/102 (96%)	95 (97%)	3 (3%)	35	39
1	D	87/102 (85%)	82 (94%)	5 (6%)	18	17
1	F	97/102 (95%)	92 (95%)	5 (5%)	21	20
1	G	87/102 (85%)	82 (94%)	5 (6%)	18	17
1	H	86/102 (84%)	82 (95%)	4 (5%)	23	24
1	I	93/102 (91%)	81 (87%)	12 (13%)	4	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	92/102 (90%)	87 (95%)	5 (5%)	20	18
1	K	86/102 (84%)	82 (95%)	4 (5%)	23	24
1	L	96/102 (94%)	92 (96%)	4 (4%)	26	28
2	E	97/102 (95%)	91 (94%)	6 (6%)	16	14
All	All	1093/1224 (89%)	1030 (94%)	63 (6%)	18	16

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31[A]	SER
1	A	63	LEU
1	A	113	LEU
1	B	0	SER
1	B	15	ILE
1	B	17	LYS
1	B	18	LYS
1	B	36	ARG
1	B	53	VAL
1	B	113	LEU
1	C	18	LYS
1	C	49	ARG
1	C	109	LYS
1	D	31	SER
1	D	79	GLU
1	D	90	LYS
1	D	109	LYS
1	D	113	LEU
2	E	39	GLN
2	E	49	ARG
2	E	90	LYS
2	E	109	LYS
2	E	113	GLU
2	E	114	GLU
1	F	36	ARG
1	F	38	VAL
1	F	63	LEU
1	F	106	GLU
1	F	113	LEU
1	G	18	LYS
1	G	31	SER
1	G	36	ARG

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Mol	Chain	Res	Type
1	G	66	LYS
1	G	79	GLU
1	H	21	SER
1	H	56	ILE
1	H	103	ARG
1	H	105	LYS
1	I	11	GLU
1	I	14	GLU
1	I	18	LYS
1	I	26	VAL
1	I	42	ILE
1	I	44	GLU
1	I	47	ARG
1	I	56	ILE
1	I	82	ARG
1	I	106	GLU
1	I	112	LEU
1	I	113	LEU
1	J	1	MET
1	J	47	ARG
1	J	55	LEU
1	J	103	ARG
1	J	109	LYS
1	K	11	GLU
1	K	17	LYS
1	K	54	ASP
1	K	90	LYS
1	L	17	LYS
1	L	31	SER
1	L	42	ILE
1	L	52	ILE

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

Mol	Chain	Res	Type
1	C	80	ASN
1	D	80	ASN
2	E	39	GLN
2	E	80	ASN
1	F	85	ASN
1	G	80	ASN
1	I	80	ASN

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Mol	Chain	Res	Type
1	K	85	ASN
1	L	85	ASN

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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
3	ACT	A	1117	-	3,3,3	0.87	0	3,3,3	0.77	0
4	ADP	L	1114	-	28,29,29	1.64	5 (17%)	43,45,45	1.88	9 (20%)
4	ADP	B	1115	-	28,29,29	1.53	5 (17%)	43,45,45	1.79	9 (20%)
3	ACT	H	1113	-	3,3,3	0.71	0	3,3,3	0.80	0
4	ADP	J	1115	-	28,29,29	1.53	5 (17%)	43,45,45	1.79	8 (18%)
3	ACT	E	1116	-	3,3,3	0.69	0	3,3,3	0.85	0
5	AMP	E	1115	-	25,25,25	1.54	4 (16%)	37,38,38	2.05	10 (27%)
3	ACT	J	1116	-	3,3,3	0.91	0	3,3,3	0.76	0
3	ACT	A	1116	-	3,3,3	0.92	0	3,3,3	0.80	0
4	ADP	I	1115	-	28,29,29	1.39	4 (14%)	43,45,45	1.89	10 (23%)

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
4	ADP	L	1114	-	-	1/16/32/32	0/3/3/3
4	ADP	B	1115	-	-	0/16/32/32	0/3/3/3
4	ADP	J	1115	-	-	2/16/32/32	0/3/3/3
5	AMP	E	1115	-	-	2/10/26/26	0/3/3/3
4	ADP	I	1115	-	-	2/16/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1115	AMP	C5-C4	5.38	1.48	1.39
4	J	1115	ADP	C5-C4	4.98	1.48	1.39
4	L	1114	ADP	C5-C4	4.82	1.47	1.39
4	B	1115	ADP	C5-C4	4.74	1.47	1.39
4	I	1115	ADP	C5-C4	4.50	1.47	1.39
4	L	1114	ADP	PA-O3A	4.44	1.64	1.59
4	J	1115	ADP	PA-O3A	3.27	1.63	1.59
4	B	1115	ADP	PA-O3A	3.26	1.63	1.59
4	L	1114	ADP	C5-N7	-2.77	1.34	1.39
4	B	1115	ADP	C5-C6	2.76	1.48	1.41
4	I	1115	ADP	PA-O3A	2.64	1.62	1.59
5	E	1115	AMP	C8-N7	2.64	1.36	1.31
5	E	1115	AMP	C5-C6	2.58	1.48	1.41
4	J	1115	ADP	C5-N7	-2.50	1.34	1.39
4	B	1115	ADP	C5-N7	-2.49	1.34	1.39
4	I	1115	ADP	C5-N7	-2.45	1.34	1.39
4	L	1114	ADP	C8-N7	2.28	1.36	1.31
4	J	1115	ADP	C5-C6	2.27	1.47	1.41
4	L	1114	ADP	C5-C6	2.27	1.47	1.41
4	I	1115	ADP	C5-C6	2.24	1.47	1.41
4	B	1115	ADP	C8-N7	2.24	1.36	1.31
5	E	1115	AMP	C5-N7	-2.15	1.35	1.39
4	J	1115	ADP	C8-N7	2.11	1.35	1.31

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1115	ADP	C5-C4-N3	-5.95	118.53	126.72
4	B	1115	ADP	C5-C4-N3	-5.95	118.53	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1115	ADP	C5-C4-N3	-5.46	119.19	126.72
5	E	1115	AMP	C5-C4-N3	-5.44	119.23	126.72
4	L	1114	ADP	C5-C4-N3	-5.27	119.47	126.72
4	J	1115	ADP	N3-C4-N9	5.26	136.10	127.17
4	I	1115	ADP	N3-C4-N9	4.95	135.59	127.17
4	L	1114	ADP	N3-C4-N9	4.93	135.56	127.17
5	E	1115	AMP	N3-C4-N9	4.70	135.16	127.17
4	B	1115	ADP	N3-C4-N9	4.57	134.95	127.17
4	I	1115	ADP	N3-C2-N1	-3.98	122.56	128.58
5	E	1115	AMP	N3-C2-N1	-3.96	122.58	128.58
4	B	1115	ADP	C2-N3-C4	3.82	121.15	111.83
4	L	1114	ADP	C4-N9-C8	3.71	109.63	105.74
5	E	1115	AMP	C2-N3-C4	3.71	120.88	111.83
4	I	1115	ADP	C2-N3-C4	3.62	120.67	111.83
4	L	1114	ADP	N3-C2-N1	-3.58	123.17	128.58
4	B	1115	ADP	N3-C2-N1	-3.56	123.19	128.58
4	L	1114	ADP	C2-N3-C4	3.47	120.30	111.83
4	J	1115	ADP	N3-C2-N1	-3.42	123.40	128.58
4	J	1115	ADP	C2-N3-C4	3.40	120.14	111.83
4	B	1115	ADP	C4-C5-N7	-3.22	106.89	110.58
4	I	1115	ADP	C4-N9-C8	2.83	108.71	105.74
4	L	1114	ADP	N9-C8-N7	-2.79	109.98	113.94
5	E	1115	AMP	C2'-C1'-N9	-2.78	106.40	113.30
5	E	1115	AMP	C4-N9-C8	2.72	108.60	105.74
4	L	1114	ADP	C5-N7-C8	2.72	107.72	103.45
5	E	1115	AMP	C2-N1-C6	2.57	122.95	118.73
5	E	1115	AMP	O3P-P-O2P	2.57	117.44	107.80
5	E	1115	AMP	C4-C5-N7	-2.54	107.67	110.58
4	L	1114	ADP	C4-C5-N7	-2.54	107.68	110.58
4	J	1115	ADP	C4-N9-C8	2.53	108.40	105.74
4	I	1115	ADP	C2-N1-C6	2.37	122.62	118.73
4	L	1114	ADP	C2-N1-C6	2.33	122.55	118.73
4	J	1115	ADP	C2-N1-C6	2.31	122.53	118.73
4	B	1115	ADP	C5-N7-C8	2.29	107.04	103.45
4	J	1115	ADP	C4-C5-N7	-2.28	107.98	110.58
4	I	1115	ADP	C4-C5-N7	-2.27	107.99	110.58
4	I	1115	ADP	N6-C6-N1	2.24	123.37	118.38
4	J	1115	ADP	C3'-C2'-C1'	2.23	105.68	101.46
4	I	1115	ADP	O3B-PB-O2B	2.23	116.15	107.80
4	B	1115	ADP	C3'-C2'-C1'	2.21	105.64	101.46
5	E	1115	AMP	O4'-C4'-C5'	2.14	116.18	109.33
4	I	1115	ADP	C5-N7-C8	2.11	106.77	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1115	ADP	C2-N1-C6	2.04	122.08	118.73
4	B	1115	ADP	C4-N9-C8	2.03	107.87	105.74

There are no chirality outliers.

All (7) torsion outliers are listed below:

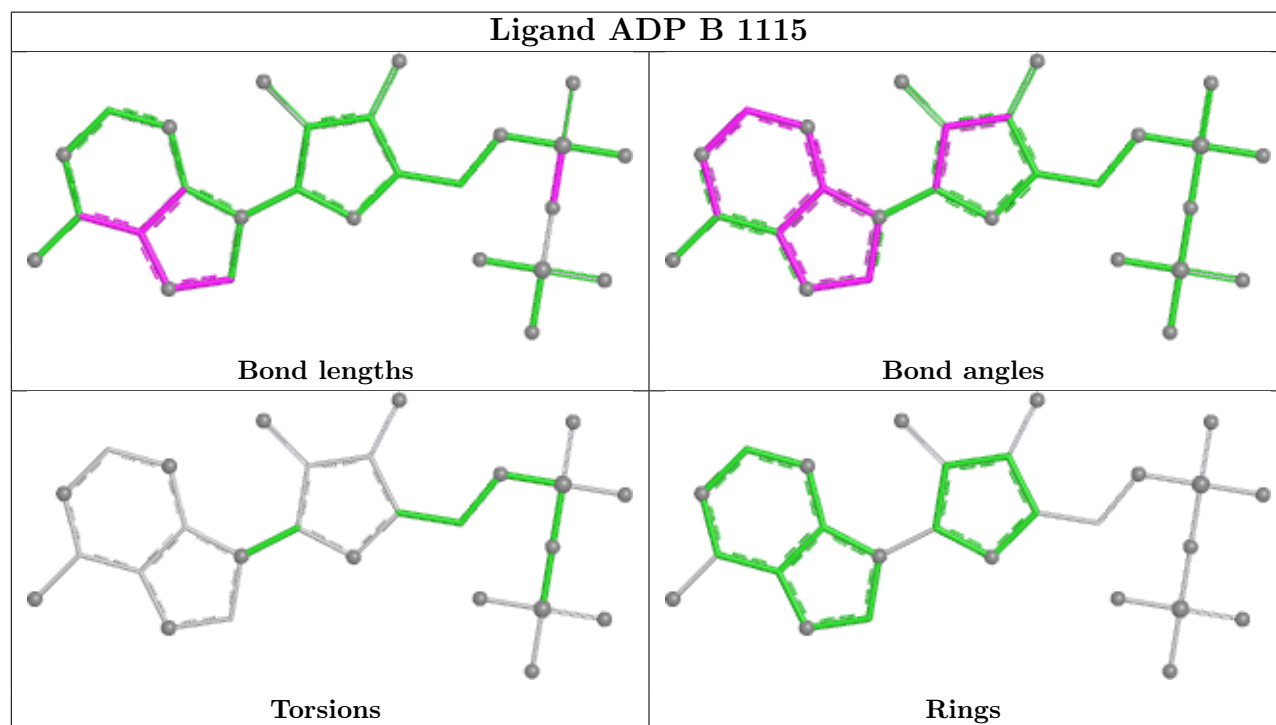
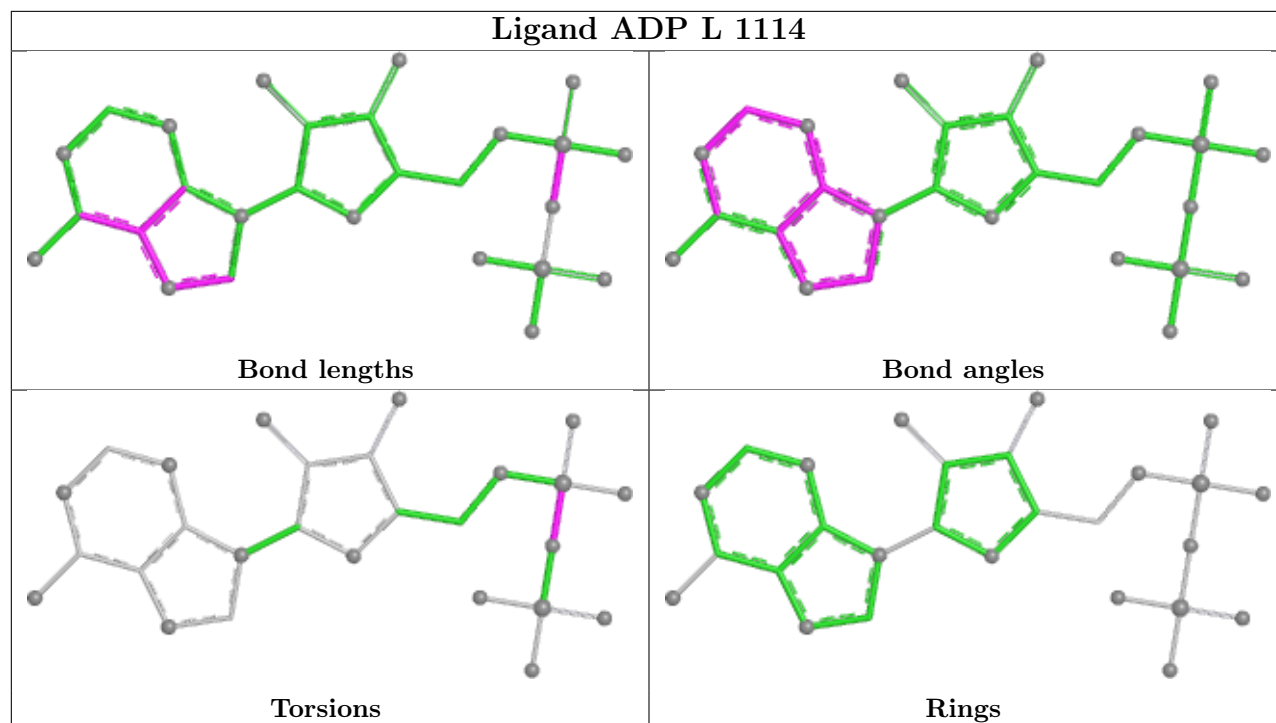
Mol	Chain	Res	Type	Atoms
4	I	1115	ADP	O4'-C4'-C5'-O5'
4	J	1115	ADP	PB-O3A-PA-O5'
5	E	1115	AMP	O4'-C4'-C5'-O5'
4	I	1115	ADP	C3'-C4'-C5'-O5'
5	E	1115	AMP	C3'-C4'-C5'-O5'
4	L	1114	ADP	PB-O3A-PA-O2A
4	J	1115	ADP	O4'-C4'-C5'-O5'

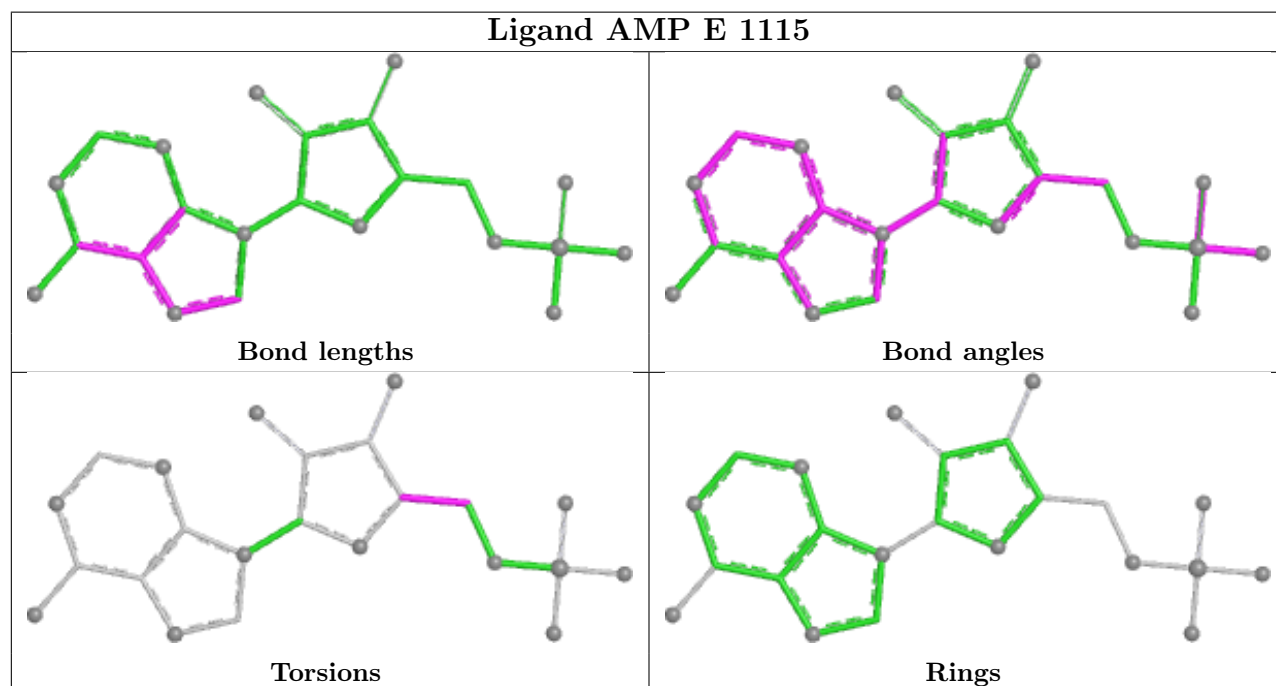
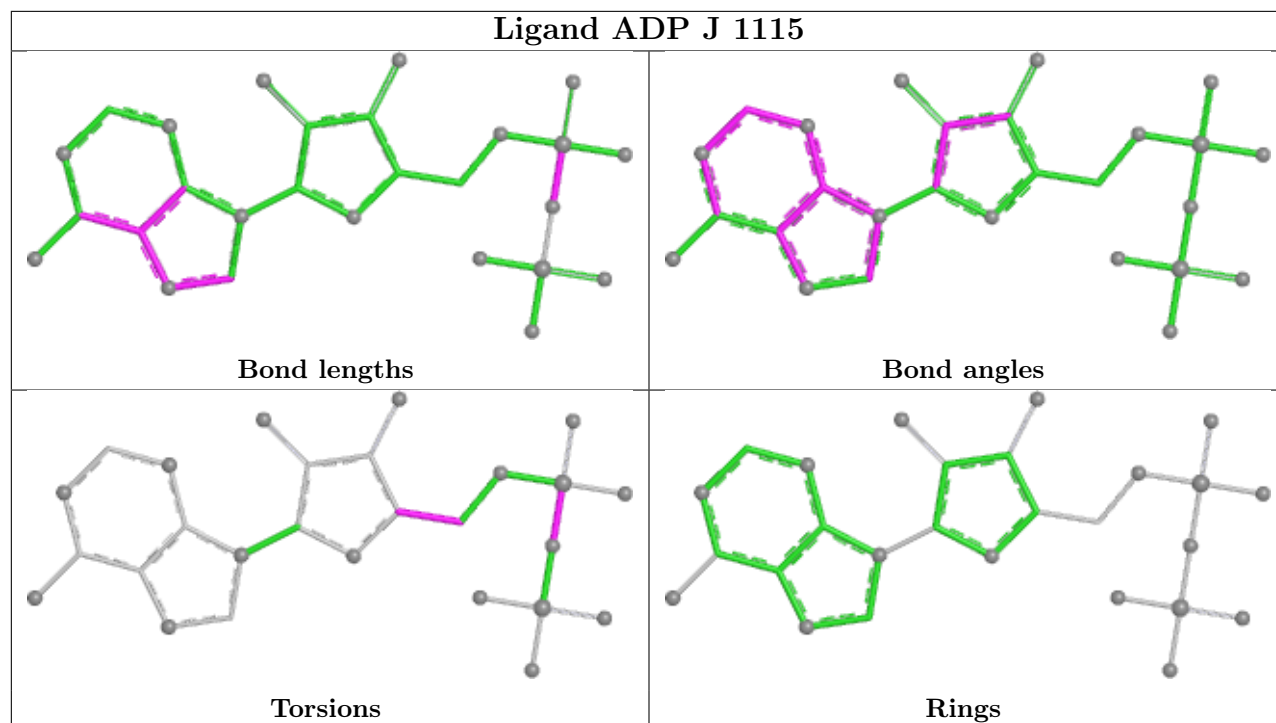
There are no ring outliers.

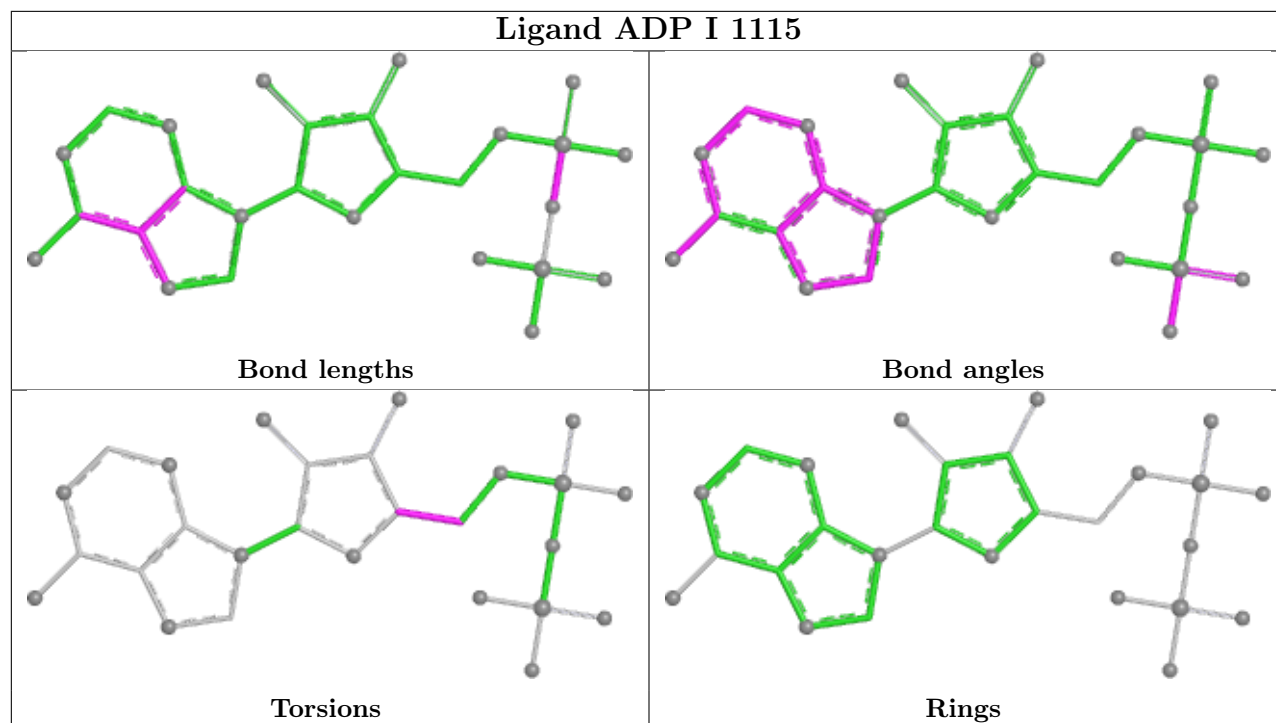
8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1117	ACT	3	0
4	B	1115	ADP	1	0
3	H	1113	ACT	4	0
4	J	1115	ADP	1	0
3	E	1116	ACT	7	0
5	E	1115	AMP	3	0
3	J	1116	ACT	3	0
3	A	1116	ACT	6	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.