wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:55 AM GMT

PDB ID	:	2J9D
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

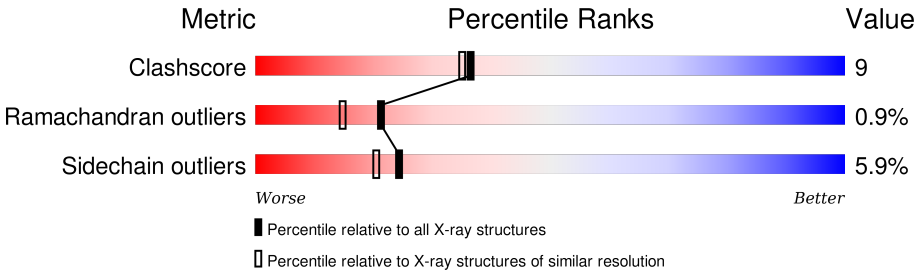
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

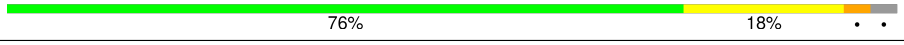
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	72% 12% • 14%
1	B	119	72% 11% • • 13%
1	C	119	76% 20% • •
1	D	119	69% 18% 13%
1	F	119	82% 10% • • 5%
1	G	119	75% 11% • 13%
1	H	119	72% 12% • 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	119	
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			

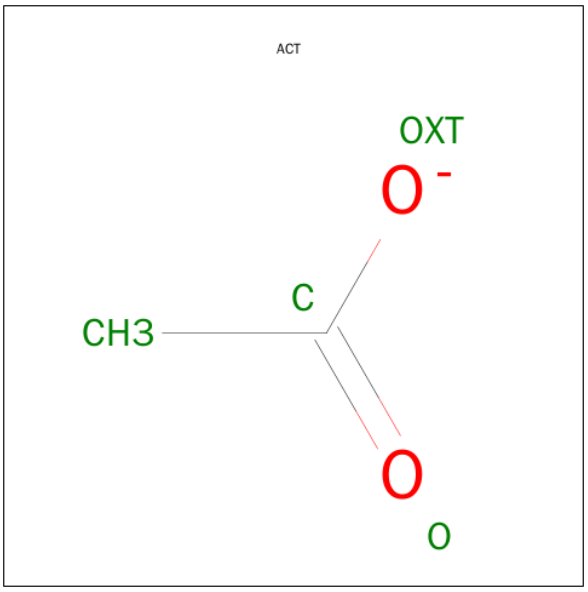
- Molecule 2 is a protein called HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059.

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:

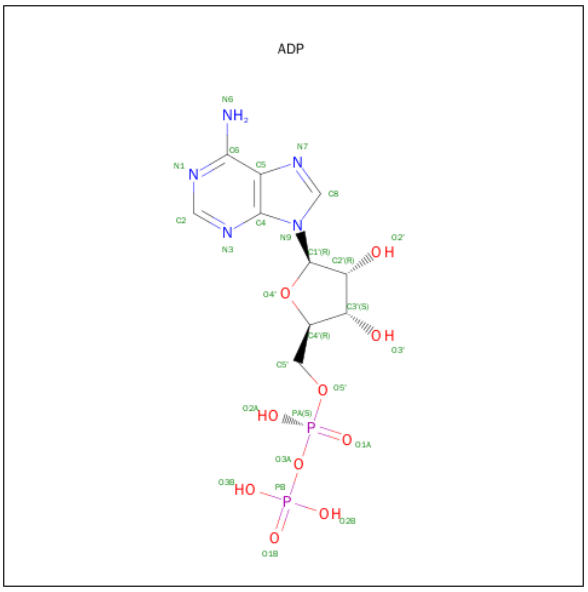
Chain	Residue	Modelled	Actual	Comment	Reference
E	113	GLU	LEU	CONFLICT	UNP Q60381

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



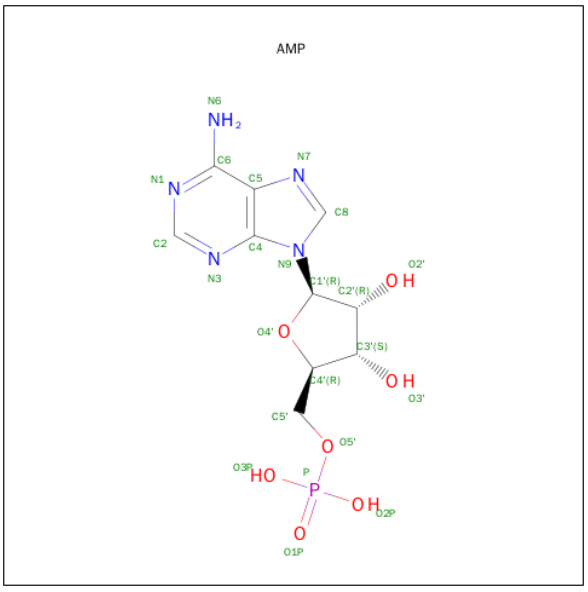
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0

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



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

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: 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 (three-letter code: 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		

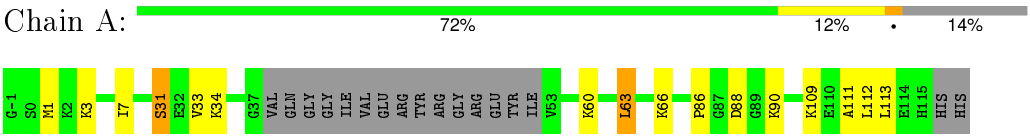
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

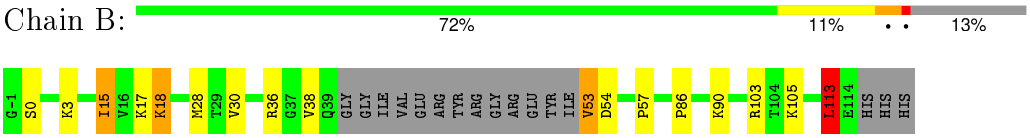
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain A:



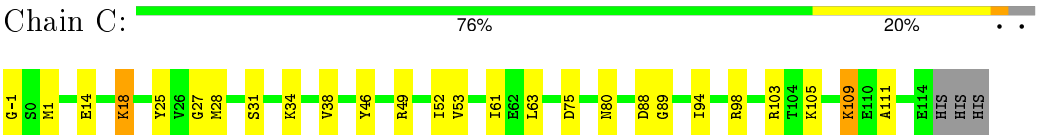
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain B:



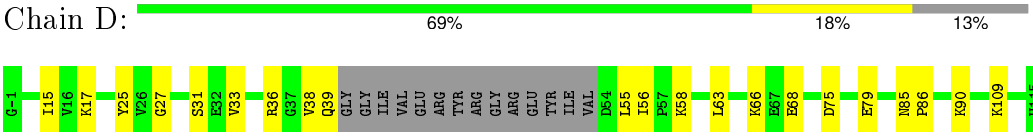
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain C:



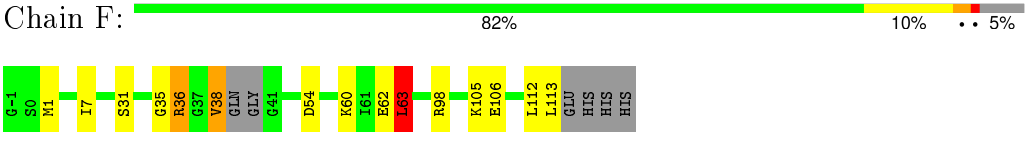
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain D:



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

Chain F:



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

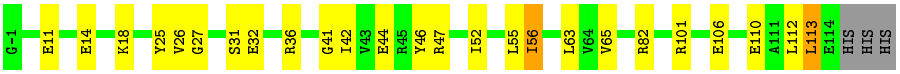
Chain G:

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

Chain H:

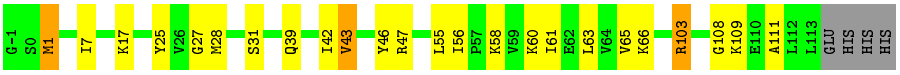
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain I:



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

Chain J:

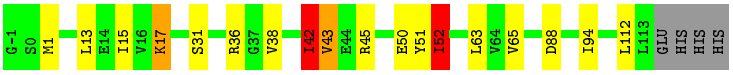


• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain K:

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

Chain L:



• Molecule 2: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain E:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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: AMP, CL, ADP, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.61	0/783	0.73	1/1049 (0.1%)
1	B	0.60	0/792	0.71	0/1062
1	C	0.56	0/904	0.71	0/1212
1	D	0.61	0/794	0.74	0/1064
1	F	0.56	0/886	0.72	1/1187 (0.1%)
1	G	0.61	0/788	0.77	2/1057 (0.2%)
1	H	0.61	0/776	0.68	0/1040
1	I	0.57	0/880	0.68	0/1182
1	J	0.58	0/876	0.70	0/1175
1	K	0.65	0/783	0.76	0/1049
1	L	0.56	0/894	0.74	0/1199
2	E	0.62	0/902	0.73	0/1210
All	All	0.59	0/10058	0.72	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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	LEU	CA-CB-CG	5.96	129.00	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	36	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	G	63	LEU	CA-CB-CG	5.36	127.62	115.30
1	F	63	LEU	CA-CB-CG	5.07	126.95	115.30

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	13	0
1	C	897	0	952	34	0
1	D	789	0	834	16	0
1	F	880	0	941	14	0
1	G	784	0	839	15	0
1	H	772	0	828	15	0
1	I	874	0	910	23	0
1	J	870	0	913	25	0
1	K	779	0	827	28	0
1	L	887	0	942	23	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	5	0
3	J	4	0	3	4	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

Continued on next page...

Continued from previous page...

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	1	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	0	0
7	K	45	0	0	0	0
7	L	73	0	0	1	0
All	All	10840	0	10654	197	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 9.

The worst 5 of 197 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:HZ2	3:H:1113:ACT:H1	1.07	1.10
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:L:42:ILE:HA	1:L:43:VAL:CB	2.00	0.89

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	98/119 (82%)	98 (100%)	0	0	100	100
1	B	99/119 (83%)	98 (99%)	0	1 (1%)	19	13
1	C	114/119 (96%)	113 (99%)	1 (1%)	0	100	100
1	D	99/119 (83%)	96 (97%)	2 (2%)	1 (1%)	19	13
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%)	19	13
1	I	114/119 (96%)	109 (96%)	4 (4%)	1 (1%)	21	15
1	J	113/119 (95%)	109 (96%)	2 (2%)	2 (2%)	11	5
1	K	98/119 (82%)	96 (98%)	1 (1%)	1 (1%)	19	13
1	L	113/119 (95%)	106 (94%)	3 (3%)	4 (4%)	4	1
2	E	114/119 (96%)	111 (97%)	2 (2%)	1 (1%)	21	15
All	All	1267/1428 (89%)	1234 (97%)	21 (2%)	12 (1%)	21	15

5 of 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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	86/102 (84%)	83 (96%)	3 (4%)	43	44
1	B	88/102 (86%)	81 (92%)	7 (8%)	15	11
1	C	98/102 (96%)	94 (96%)	4 (4%)	37	36
1	D	87/102 (85%)	83 (95%)	4 (5%)	33	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	97/102 (95%)	91 (94%)	6 (6%)	23 19
1	G	87/102 (85%)	83 (95%)	4 (5%)	33 31
1	H	86/102 (84%)	83 (96%)	3 (4%)	43 44
1	I	93/102 (91%)	82 (88%)	11 (12%)	6 3
1	J	92/102 (90%)	87 (95%)	5 (5%)	27 24
1	K	86/102 (84%)	82 (95%)	4 (5%)	32 30
1	L	96/102 (94%)	91 (95%)	5 (5%)	29 25
2	E	97/102 (95%)	89 (92%)	8 (8%)	14 10
All	All	1093/1224 (89%)	1029 (94%)	64 (6%)	24 20

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	63	LEU
1	G	79	GLU
1	L	17	LYS
1	F	98	ARG
1	G	18	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	80	ASN
1	F	80	ASN
1	J	80	ASN
2	E	39	GLN
1	H	80	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 carbohydrates 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	1116	-	1,3,3	0.54	0	0,3,3	0.00	-
3	ACT	A	1117	-	1,3,3	0.88	0	0,3,3	0.00	-
4	ADP	B	1115	-	22,29,29	1.09	2 (9%)	27,45,45	1.86	3 (11%)
5	AMP	E	1115	-	20,25,25	1.22	2 (10%)	22,38,38	2.45	4 (18%)
3	ACT	E	1116	-	1,3,3	0.62	0	0,3,3	0.00	-
3	ACT	H	1113	-	1,3,3	0.42	0	0,3,3	0.00	-
4	ADP	I	1115	-	22,29,29	1.00	1 (4%)	27,45,45	2.13	5 (18%)
4	ADP	J	1115	-	22,29,29	1.12	2 (9%)	27,45,45	1.73	2 (7%)
3	ACT	J	1116	-	1,3,3	0.63	0	0,3,3	0.00	-
4	ADP	L	1114	-	22,29,29	1.11	2 (9%)	27,45,45	1.86	3 (11%)

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
3	ACT	A	1116	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1117	-	-	0/0/0/0	0/0/0/0
4	ADP	B	1115	-	-	0/12/32/32	0/3/3/3
5	AMP	E	1115	-	-	0/6/26/26	0/3/3/3
3	ACT	E	1116	-	-	0/0/0/0	0/0/0/0
3	ACT	H	1113	-	-	0/0/0/0	0/0/0/0
4	ADP	I	1115	-	-	0/12/32/32	0/3/3/3
4	ADP	J	1115	-	-	0/12/32/32	0/3/3/3
3	ACT	J	1116	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	L	1114	-	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1114	ADP	O4'-C1'	2.14	1.43	1.41
4	B	1115	ADP	O4'-C1'	2.35	1.44	1.41
4	J	1115	ADP	O4'-C1'	2.35	1.44	1.41
5	E	1115	AMP	O4'-C1'	2.63	1.44	1.41
4	I	1115	ADP	C5-C4	2.93	1.47	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1115	ADP	N3-C2-N1	-8.27	122.56	128.89
5	E	1115	AMP	N3-C2-N1	-8.24	122.58	128.89
4	L	1114	ADP	N3-C2-N1	-7.48	123.17	128.89
4	B	1115	ADP	N3-C2-N1	-7.46	123.19	128.89
4	J	1115	ADP	N3-C2-N1	-7.18	123.40	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 30 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.